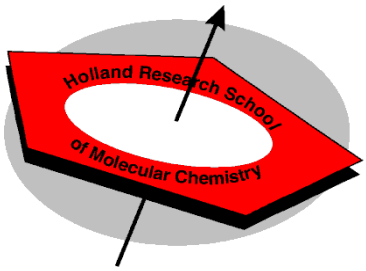
Holland Research School of Molecular Chemistry



Annual Report 2011

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Holland Research School of Molecular Chemistry

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Content

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 2011. 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). In 2011, the HRSMC was visited by a Peer Review Committee in order to apply for re-accreditation for the period 2012 – 2018. 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). 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 2011, 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. R. 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.

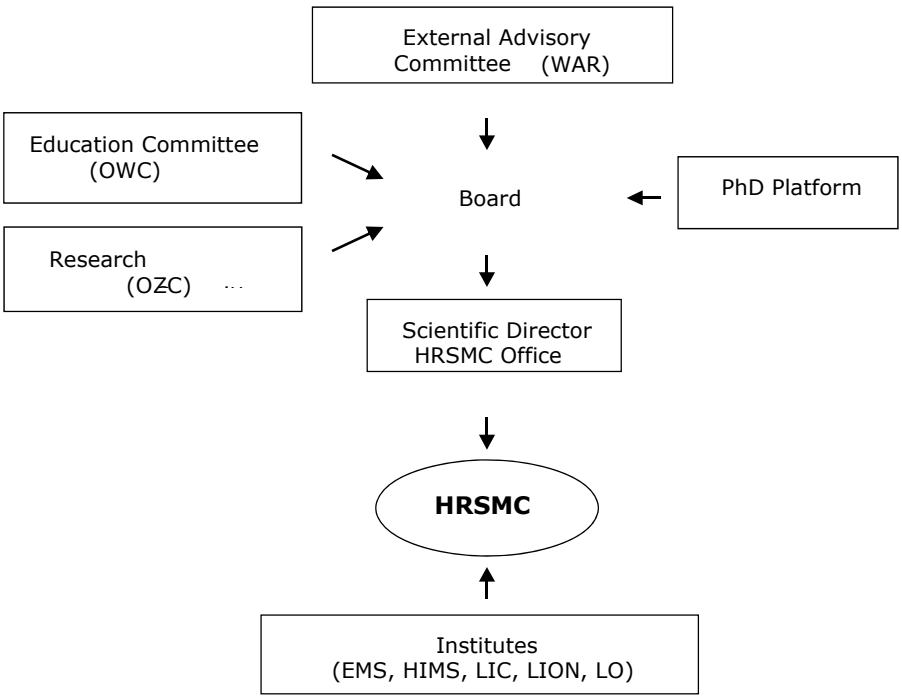


Figure 1.1 Schematic organisation of the HRSMC

On December 31, 2011 about 220 persons were employed within the HRSMC (several are not full-time involved in research, for details see Annex 4.3).

1.3 General Activities and Headlines of 2011

In 2011, 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 2011:

- The annual HRMSC Symposium was held at the VU University on November 4. Following the advice of the Education Committee and the PhD platform, the same format of last year symposium was used 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. P. Gros (UU) and PhD student S. Roters (WWU Münster), there were lectures of three PhD students and four lectures by senior scientists. Furthermore, the Dick Stufkens prize was awarded to Dr. S. Ioppolo (UL), 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 45 posters, mainly presented by PhD students. Further details regarding this symposium can be found in Chapter 3.2.

- The HRSMC educational activities of 2011 consisted of:
  - The two weeks Course '*Molecular Simulation*', organised under the auspices of CECAM (January 3-14 2011, UvA)
  - The HRSMC Course '*Physical Methods in Inorganic Chemistry*' (Jan. 24, 28, 31 and Feb. 1, UvA/UL)

In addition to these Courses, the following special activities were organized:
- 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*'.
- Following the advice of the Education Committee, the first HRSMC lab visit within Research Theme 2 (Photochemistry and (Laser) Spectroscopy) was organized at the UL on January 25. Four HRSMC research groups were visited by PhD students, postdocs and staff members from other UL, VU and UvA HRSMC groups. As within research theme 2 a lot of specialized equipment is used, this lab visits were organized to share expertise and knowledge, and to stimulate collaboration. The next lab visit will take place at the UvA/VU in 2013.
- Following the advice of the PhD platform, an Introduction Event for first-year PhD students as well as a Social Event for all HRSMC members was organized on June 9. At the Introduction Event several Board members and members of the Education Committee gave an overview of the research and educational activities within the HRSMC. The Social Event, a soccer tournament and some games, was organized by PhD students and the HRSMC, as a networking activity between UvA, UL and VU PhD students.

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 2011 described above.

Research highlights

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

- Dr. S. Ioppolo (UL) received the HRSMC annual Dick Stufkens Prize for the most outstanding PhD thesis within HRSMC.
- Science Park New Ideas Competition 2011 won by Hong Zhang (Molecular Photonics, UvA) and Maurice Aalders (AMC) for the development of a catheter that is able to detect microbial infections at an early stage.
- The Dutch Scientific Organization NWO grants ECHO projects to pursue high quality, challenging scientific ideas that open new research areas and establish scientific innovation. The following HRSMC staff members received a NWO-ECHO grant:
    - Andreas Ehlers (VU) for the development of the next generation of (chiral) pentaorganosilicates.
    - Francesco Buda (UL) grant for his proposal entitled "Bio-inspired molecular rectifier for artificial photosynthesis".
    - Evert-Jan Baerends/Oleg Gritsenko (VU) for the proposal "Novel density-matrix response functional theory to calculate molecular electronic excitations including double, bond-breaking, and charge-transfer excitations"
    - Sander Woutersen (UvA) for the project entitled “Slippery when wet. How water lubricates molecular machines”
    - Wybren Jan Buma (UvA) for his “Molecular machines at work in the gas phase” project.

VENI, VIDI, VICI grants:
In October, Dr. A.J. (Aurora) Cruz-Cabeza (UvA, Computational Chemistry) received a VENI grant, as well as Dr. D. Millo (for his work at VU, Biomolecular Analysis and Spectroscopy)

Publications from all HRSMC research groups published in 2011, can be found in Annex 4.4. Many of these publications appeared in high-impact journals, such as for example:

- Haud, N.; Kara, F.; Diekmann, S.; Henneke, M.; Willer, J.R.; Hillwig, M.S.; Gregg, R.G.; MacIntosh, G.C.; Gartner, J.; Alia, A.; Hurlstone, A.F.L.; rnaset2 mutant zebrafish model familial cystic leukoencephalopathy and reveal a role for RNase T2 in degrading ribosomal RNA, *Proc. Natl. Acad. Sci. USA* **2011,** *108*, 1099.

- Song, C.; Psakis, G.; Lang, C.; Mailliet, J.; Gartner, W.; Hughes, J.; Matysik, J.; Two ground state isoforms and a chromophore D-ring photoflip triggering extensive intramolecular changes in a canonical phytochrome, *Proc. Natl. Acad. Sci. USA* **2011,** *108*, 3842.

- Bonnet, S.; Limburg, B.; Meeldijk, J.D.; Klein Gebbink, R.J.M.; Killian, J.A.; Ruthenium-Decorated Lipid Vesicles: Light-Induced Release of Ru(terpy)(bpy)$(OH_2)^{2+}$ and Thermal Back Coordination, *J. Am. Chem. Soc.* **2011,** *133*, 252-261.

- Cavarzan, A.; Scarso, A.*; Sgarbossa, P.; Strukul, G.; Reek, J.N.H.*; Supramolecular Control on Chemo- and Regioselectivity via Encapsulation of (NHC)-Au Catalyst within a Hexameric Self-Assembled Host, *J. Am. Chem. Soc.* **2011**, *133*, 2848-2851.

- Dydio, P.; Rubay, C.; Gadzikwa, T.; Lutz, M.; Reek, J.N.H.*; Cofactor-Controlled Enantioselective Catalysis, *J. Am. Chem. Soc.* **2011**, *133, in press* highlighted in C&E News and C2W.

- Dunbar, R.C.; Steill, J.D.; Oomens, J.; Chirality-induced conformational preferences in peptide-metal ion binding revealed by IR spectroscopy, *J. Am. Chem. Soc.* **2011**, *133*, 1212-1215.

- Dunbar, R.C.; Steill, J.D.; & Oomens, J.; Encapsulation of metal cations by the PhePhe ligand: a cation-pi ion cage, *J. Am. Chem. Soc.* **2011**, *133*, 9376-9386.

- Lyaskovskyy, V.; Elders, N.; Ehlers, A.W.; Lutz, M.; Slootweg, J. C.; Lammertsma, K.; Remarkable metal-complexed phosphorus analogues of the cyclopropenyl-carbene–cyclobutadiene rearrangement, *J. Am. Chem. Soc.* **2011**, *133*, 9704-9707.

Personnel mutations

At the Institute for Electrons and Molecular Structure (EMS) of the Vrije Universiteit (VU):
- In June 2011, Prof. dr C. Gooijer (VU) had his official emeritate.

At the van 't Hoff Institute of Molecular Chemistry (HIMS) of the Universiteit van Amsterdam (UvA), in the group of Computational Chemistry & Physics:
- As of January 1, Dr. B. Ensing has been appointed as assistant professor.
- As of October 1, Dr. J. Vreede has been appointed as assistant professor.
- As of July 1, Prof. dr. E.J. Meijer has been appointed as professor.

At the Leiden Institute of Chemistry (LIC), Leiden Observatory (LO) and the Leiden Institute of Physics (LION) of the Universiteit Leiden (UL):
- As of June 1, Prof. dr. H. Linnartz has been appointed as professor at the Raymond and Beverly Sackler Laboratory for Astrophysics
- As of July 1, Dr. J. Neugebauer has been appointed as professor at the Technical University Braunschweig. With this appointment, the HRSMC membership of the group 'Theoretical Chemistry' ended.

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 12 joint publications in 2011, 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.

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 2011 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 2011

Theme	Group leader(s)	Institute	Workgroup
1	Bouwman[1,2]	LIC	Metals in Catalysis, Biomimetics & Inorganic Materials[3]
	Elsevier[1,2]	HIMS	Co-ordination and Organometallic Chemistry
	Hiemstra[1,2]/ Timmerman	HIMS	Synthetic Organic Chemistry
	Lammertsma[2]	EMS	Organic and Organometallic Chemistry
	Orru[2]	EMS	Synthetic and Bio-organic Chemistry
	Overkleeft/vd Marel	LIC	Bio-organic Synthesis
	Reek[1,2]/Hartl	HIMS	Supramolecular Catalysis
	Wever[1,2]	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[1,2]	LIC	Surface Chemistry and Catalysis
	Linnartz	LO	Laboratory Astrophysics and Astrochemistry
3	Bickelhaupt[1,2]/ Visscher	EMS	Theoretical Chemistry
	Bolhuis/Meijer	HIMS	Computational Chemistry & Physics
	Neugebauer	LIC	Theoretical Chemistry

[1]also NIOK; [2]also NRSC-Catalysis;

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** 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 novel classes of organophosphorous compounds in the context of sustainability, using novel Al,P- and B.P-based frustrated Lewis pairs (FLPs) and P-based metal-template directed methods akin to the Fischer and Schrock carbene complexes. The designs are supported by DFT calculations. 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 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 tools for transition metal catalysis, based on rational ligand design, supramolecular concepts and bioinspired approaches. With these new tools new and existing reactions are developed with a focus on high atom-efficiency, control of chemo-, regio-, and stereo-selectivity, and optimized activity and stability of the catalyst. In addition to development of novel reaction relevant for biorenewable conversion, we also study reaction for green energy applications (water oxidation, proton reduction, formic acid decomposition). In addition, new solutions to 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 of 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.

Metals in Catalysis, Biomimetics & Inorganic Materials

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

Research topics

- Inorganic chemistry
- Homogeneous- and photo-catalysis (reported within NIOK)
- Biomimetic and bioinorganic chemistry
- Molecular and solid-state materials

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. In this study, several substituted phenanthrolines have been synthesized, characterized and coordinated to Eu(III). Figure 1 shows the structure of $[Eu(2MeOphen)_2(NO_3)_3]$; in comparison with the reported $[Eu(phen)_2(NO_3)_3]$, the phenanthroline ligands are slightly twisted (N2<N1 and N4<N3), to accommodate additional Eu–O interactions.

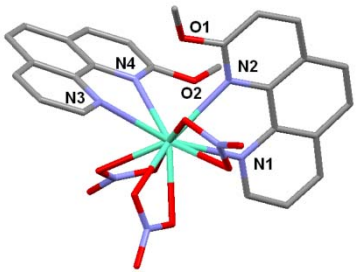


Figure 1: crystal structure of $[Eu(2MeOphen)_2(NO_3)_3]$, showing a highly non-symmetrical coordination sphere around the central europium(III) ion.

The luminescent properties have been studied of the resulting complexes with the general formula $[EuL_2(NO_3)_3]$, L=2-cyanophenanthroline, 2-chloro-phenanthroline and 2-methoxyphenanthroline. Noteworthy is the change in shape of the excitation band between 250 and 300 nm. Substitution of phenanthroline also influences the luminescence intensity, which decreases in the order –OMe > –CN > –Cl.

We also used light, in the visible region, to trigger molecular motion. Thioether-cholesterol conjugates were synthesized that bind to ruthenium complexes through their sulfur atom and intercalate into lipid bilayers through their apolar tail. Ruthenium-decorated unilamellar vesicles can be prepared, which, upon visible light irradiation, release the ruthenium complex by selective cleavage of the Ru-S coordination bond. When the lipids are negatively charged the photochemically generated aqua Ru complex stays close to the membrane and can be re-bound thermally (S. Bonnet, B. Limburg, J. Meeldijk, R. J. M. Klein Gebbink, and J. A. Killian, *J. Am. Chem. Soc.* **2011**, *133*, 252-261). We are now working on modifying the metal complex to enhance the rate of the thermal binding process to realize light-induced hopping of a molecule at the water-bilayer interface. On the other hand, with neutral lipids the aqua Ru complex diffuses away in solution, which we are currently investigating for the delivery of anticancer metallodrugs into cancer cells using visible light.

Following our discovery of the strongly cooperative spin-crossover mononuclear compounds $[Fe(bapbpy)(NCS)_2]$ (see reports of 2008 and 2009), we have been focusing on studying how modifying the tetrapyridyl bapbpy ligand modifies the spin-transition properties of its iron(II) complexes. Notably, we discovered that materials made of

isomers of the same molecule show very different spin-crossover properties, which makes material design highly challenging process (Z. Arcis-Castíllo et al, *Chem. Eur. J.* **2011**, *17,* 14826). We are pursuing this research line with the aim of obtaining molecular materials with cooperative SCO properties occurring around room temperature. In addition, in a collaboration with the CNRS in Toulouse we have studied by Raman mapping, optical microscopy (S. Bedoui et al, *Chem. Phys. Lett.* **2010**, *499*, 94), and more recently high-pressure diffraction studies at the ESRF synchrotron facility in Grenoble, the two independent spin transitions of [Fe(bapbpy)$(NCS)_2$]. This last study characterized for the first time a two-step, pressure-induced spin crossover at room temperature (H. Shepherd et al, *Phys. Rev. B* **2011**, *84*, 144107).

Key publications 2008-2011

- Mooibroek, T. J.; Schoon, L.; Bouwman, E.; Drent, E.; Carbonylation of Nitrobenzene in Methanol with Palladium Bidentate Phosphane Complexes: An Unexpectedly Complex Network of Catalytic Reactions, Centred around a Pd-imido Intermediate, *Chem.-Eur. J.* **2011,** *17*, 13318-13333.

- Bonnet, S.; Limburg, B.; Meeldijk, J. D.; Klein Gebbink, R. J. M.; Killian, J. A.; Ruthenium-Decorated Lipid Vesicles: Light-Induced Release of Ru(terpy)(bpy)$(OH_2)^{2+}$ and Thermal Back Coordination, *J. Am. Chem. Soc.* **2011,** *133*, 252-261.

- Arcis Castíllo, Z., Zheng S., Siegler M. A., Roubeau O., Bedoui S., Bonnet, S.; Tuning the transition temperature and cooperativity of bapbpy-based mononuclear spin-crossover compounds: interplay between molecular- and crystal-engineering, *Chem. Eur. J.* **2011**, *17,* 14826-14836.

Future developments

In the topic of biomimetics we plan to continue the research towards the catalytic conversion of CO_2. By varying the steric and electronic properties of the ligands, attempts are 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.

The research of Dr. Bonnet will focus on two projects in the bioinorganic topic: one aimed at controlling the motion of molecules with light, and one at the light-activation of ruthenium-based anticancer drugs. One PhD students (Azadeh Bahreman) is working on the first project. Meanwhile, the expertise in homogeneous catalysis and photochemistry of Prof. Bouwman and Dr. Bonnet are now combined within two projects on photocatalysis, with one PhD student (Bart Limburg) and two postdoctoral collaborators. Finally we also continue research in spin-transitions materials, for which a 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. Among the new ligands that are studied, the phenol-oxazolines

and pyridine-oxazolines offer ample possibilities for substitution, which allows for tuning the ligand to the acceptor levels on the lanthanide.

Co-ordination and Organometallic Chemistry

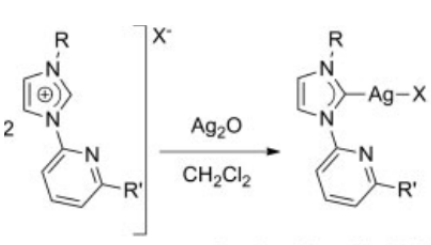
Prof.dr C.J. Elsevier

Research topics

- Organometallic and coordination chemistry
- Catalytic bond-formation and -breaking
- High-pressure NMR and transition metal NMR spectroscopy
- Heterogenization of homogeneous catalysts

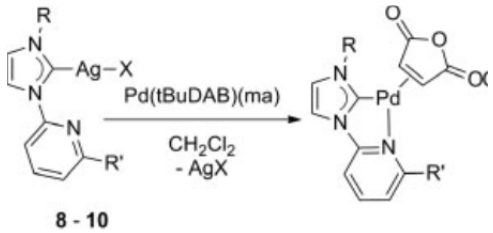
Summary of research activities

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). Other methodologies for heterogenization, immobilization and recycling of homogeneous catalysts receive ample attention.



5 - 7

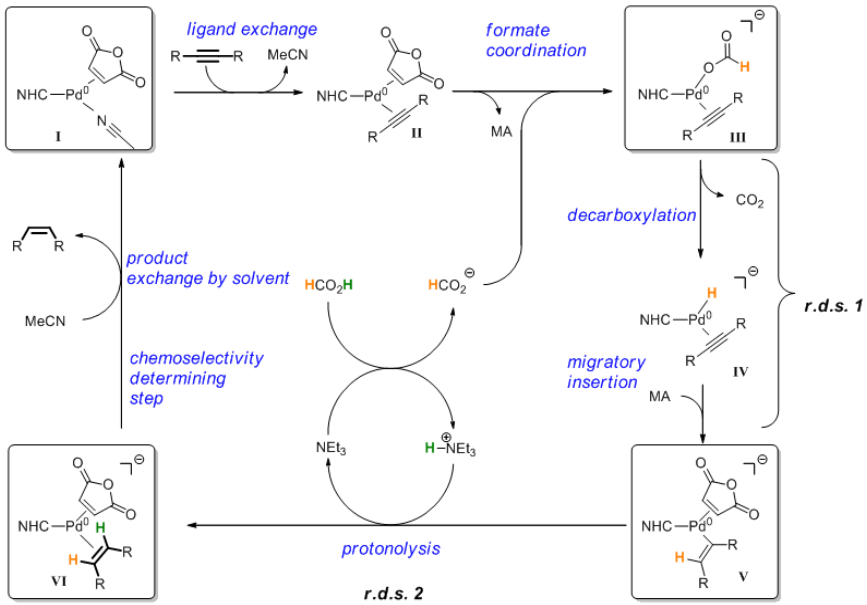
8a: R = Mes, R' = H, 89%
8b: R = Mes, R' = Me, 83%
9a: R = DiPP, R = H, 86%
9b: R = DiPP, R' = Me, 95%
10a: R = *i*Pr, R' = H, 92%
10b: R = *i*Pr, R' = Me, 88%



8 - 10

11a: R = Mes, R' = H, 96%
11b: R = Mes, R' = Me, 91%
12a: R = DiPP, R' = H, 91%
12b: R = DiPP, R' = Me, 94%
13a: R = *i*Pr, R' = H, 0%
13b: R = *i*Pr, R' = Me, 0%

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, studies revolved about palladium compounds encompassing bidentate carbene-pyridyl ligands and similar materials. These studies concern a new niche as a part of the unique (base-free) transfer-hydrogenation reaction mediated by palladium-NHC species that we discovered and about which mechanism we have published recently (*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. After obtaining insight in details of the mechanism, we have been able to provide a working catalyst that obviates the use of added base, which is based on bidentate C-N carbene-amine type ligands (see Appl. Organomet. Chem. **2011**, *25*, 276-282 and the schemes).



An interesting range of new ruthenium compounds with bidentate carbene-amine and similar ligands have been synthesized and were applied in selective hydrogenations of ketones and esters (to be published).

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. Again, we have synthesized a number of novel heterobidentate NHC ligands containing a secondary donor atom. 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 – generally weaker - secondary donor group. Varying their basicity, hence coordinative properties, leads to specific behaviour in e.g. hydrogenation reactions.
Part of this project has been carried out in collaboration with Taiwanese colleagues. 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 14 papers, one of which appeared in 2011.

This year also saw a growing interest and exciting results concerning catalyst immobilization. The progress has been good, although the number of papers was at a low (due to fast acceptance of papers there were many in 2010 and few in 2011). The officially finished NWO-NSC-project with the National Taiwan University at Taipei enjoyed new impetus in visits and the work by S. Warsink at Taipei and Bloemfontein. Soraya Sluijter joined the group as PhD student starting her work on late-transition-metal complexes of bis-carbenes in catalysis as main topic.

Future developments

The research for the immediate future will generally be aimed at design and synthesis of organometallic compounds for stoichiometric and homogeneous catalytic reactions, particularly addition of small molecules to unsaturated compounds, carbon-element bond forming and reduction 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 continued attention. Especially the immobilization of catalysts and its implications in (transfer) hydrogenations using late-transition-metal(NHC) complexes will be pursued. Furthermore, the design of (chiral) ligands will continue to be important, especially in relation to carbon-element bond forming reactions, carbonylations and related reactions.

Key publications 2008-2011

- Hauwert, P.; Maestri, G.; Sprengers, J.W.; Catellani, M.; Elsevier, C.J.; Transfer Semihydrogenation of Alkynes Catalyzed by a Zero-Valent Palladium N-Heterocyclic Carbene Complex, *Angew. Chem. Int. Ed.*, **2008**, *47*, 3223-3226.

- Hauwert, P.; Boerleider, R.; Warsink, S.; Weigand, J.J.; Elsevier, C.J.; Mechanism of Pd(NHC)-catalyzed transfer hydrogenation of alkynes, *J. Am. Chem. Soc.*, **2010**, *132*, 16900-16910.

- Warsink, S.; Bosman, S.; Weigand, J.J.; Elsevier, C.J.; Rigid pyridyl-substituted NHC-ligands, their Pd(0) complexes and their application in selective transfer semi-hydrogenation of alkynes, *Appl. Organomet. Chem.* **2011**, *25*, 276-282.

Synthetic Organic Chemistry

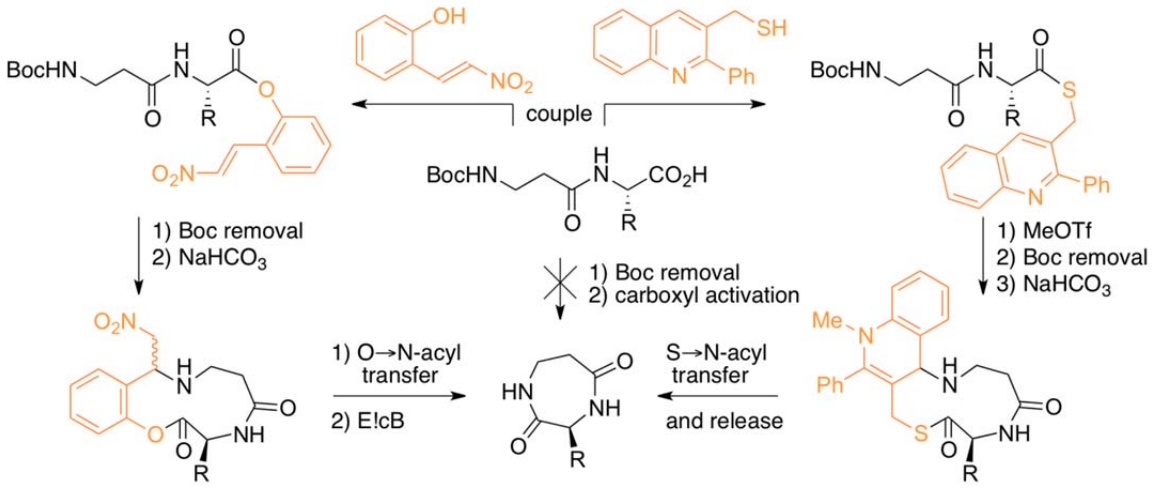
Prof. dr. H. Hiemstra, Prof. dr. P. Timmerman, Dr. J.H. van Maarseveen, Dr. S. Ingemann (UvA)

Research topics

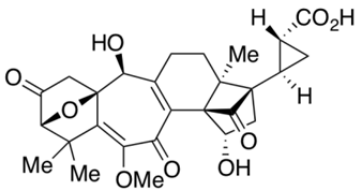
- Synthetic methodology development
- Target-oriented synthesis
- Organocatalysis
- Chemical biology

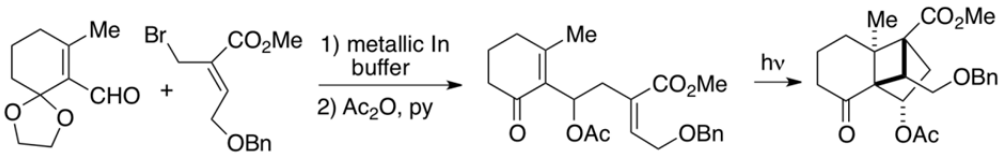
Summary of research activities

Synthetic methodology development: Due to their strained character, seven-membered bislactams are excellent targets for the development of novel and powerful lactamization methods. We have found that esterfication of *N*-terminal protected β-peptides with commercially available *o*-hydroxy-β-nitrostyrene, followed by liberation of the *N*-terminus gave the seven-membered strained bislactams in good yield. Mechanistic studies pointed to the intermediacy of an 11-membered macrocyclic intermediate, formed via an intramolecular aza-Michael reaction, which collapses to the seven-membered lactam via a ring-contractive O→N acyl-transfer reaction, followed by a retro-aza-Michael reaction liberating the lactam. In collaboration with the group of Prof. Levacher in Rouen (France) it was shown that also quinolines can be used as auxiliaries to facilitate lactamization using a similar mechanistic reaction pathway, although with less efficiency (*submitted*).

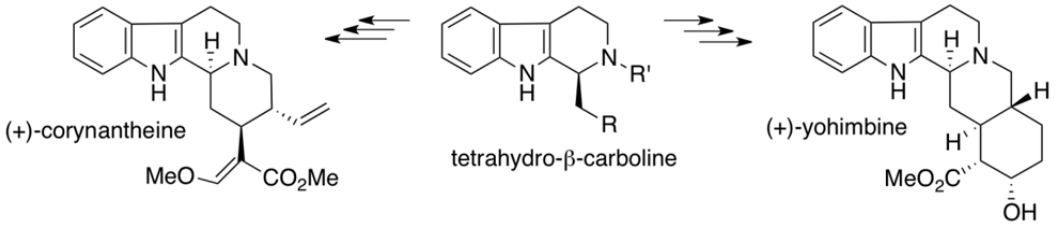


Target-oriented synthesis: In our research toward the total synthesis of the terpenoid hatching agent solanoeclepin. A very efficient and convergent synthesis of the tricyclic core was realized with all functionality in place to complete the total synthesis or simpler active analogues in order to combat potato cyst nematodes as parasites in potato production.

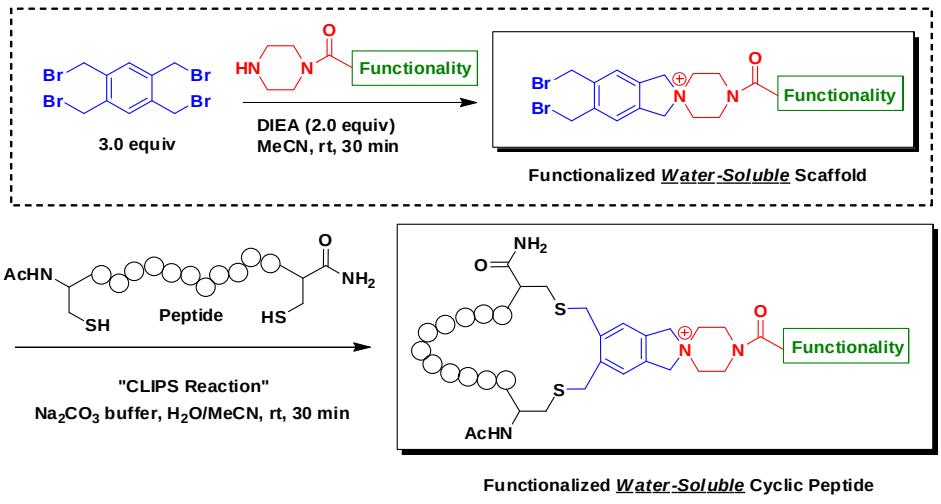

solanoeclepin A



Organocatalysis: Chiral biarylphosphoric acids were used to catalyse Pictet-Spengler reactions in order to prepare tetrahydro-β-carbolines in high ee's. Starting from these *N*-heterocycles we achieved the most efficient asymmetric total syntheses to date of indole alkaloids like (+)-corynantheine and (+)-yohimbine.



Chemical biology Water-soluble scaffolds that are based on Pepscan 's (Lelystad, The Netherlands) CLIPS-technology have been prepared that conformationally constrain side chain unprotected linear peptides containing two cysteines. These scaffolds contain functionality with orthogonal reactivity to be used for labeling and ligation. This is illustrated by the chemical ligation of two dissimilar constrained peptides via oxime-ligation or strain-promoted azide-alkyne cycloaddition in aqueous media. Such functionalized scaffolds may be used for indirect labeling, i.e. by coupling of an appropriately functionalized FLAG, biotin, fluorescein, rhodamine or luciferin tag to a cyclized peptide carrying the compatible functional group at the scaffold. Also, these scaffolds provide a general and easy applicable route toward complex water-soluble double-loop mimics of discontinuous protein binding sites and can also be used to solubilize or label cyclic peptides. The method opens new perspectives in the field of protein mimicry.



Key publications 2008-2011

- Detz, R.J.; Delville, M.M.E.; Hiemstra, H.; Van Maarseveen, J.H.; Enantioselective copper-catalyzed propargylic amination, *Angew. Chem. Int. Ed.* **2008**, *47*, 3777-3780.

- Springer, J.; De Cuba, K.R.; Calvet-Vitale, S.V.; Geenevasen, J.A.J.; Hermkens, P.H.H.; Hiemstra, H.; Van Maarseveen, J.H.; Backbone amide linker strategy for the synthesis of 1,4-triazole-containing cyclic tetra- and pentapeptides, *Eur. J. Org. Chem.* **2008**, 2592-2600.

- Wanner, M.J.; Boots, R.N.A.; Eradus, B.; De Gelder, R.; Van Maarseveen, J.H.; Hiemstra, H.; Organocatalytic enantioselective total synthesis of (-)-arboricine, *Org. Lett.* **2009**, *11*, 2579-2581.

- Nessen, M.A.; Kramer, G.; Back, J.W.; Baskin, J.M.; Smeenk, L.E.J.; De Koning, L.J.; Van Maarseveen, J.H.; De Jong, L.; Bertozzi, C.R.; Hiemstra, H.; De Koster, C.G.; Selective enrichment of azide-containing peptides from complex mixtures, *J. Proteome Res.* **2009**, *8*, 3702-3711.

- Breman, A.C.; Dijkink, J.; Van Maarseveen, J.H.; Kinderman, S.S.; Hiemstra, H.; Expedient pyrrolizidine synthesis by propargylsilane addition to *N*-acyliminium ions followed by gold-catalyzed α-allenyl amides cyclization, *J. Org. Chem.* **2009**, *74*, 6327-6330.

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 and a cyclic tetrapeptide. Our future research will also focus on novel catalytic methods to make activated peptide aryl esters. Initial experiments have shown that peptide arylesters may be prepared without any sign of epimerization by the Cu(II)-catalyzed reaction between peptides and arylboroxines (based on the recently discovered Chan-Lam reaction). In the following year(s) the Chan-Lam esterification approach will be extended to the previously developed lactamization auxiliaries. Next to the strained lactams, a new research line has been started to develop a general synthetic approach towards the natural lasso peptide series.

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

Organic and Organometallic 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 is becoming scarce 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 phosphaalkenes. 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 phospha-scorpionate catalysts. We showed phosphaalkynes (P≡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 new classes of P/Al- and P/B- based Frustrated Lewis Pairs, and develop 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.

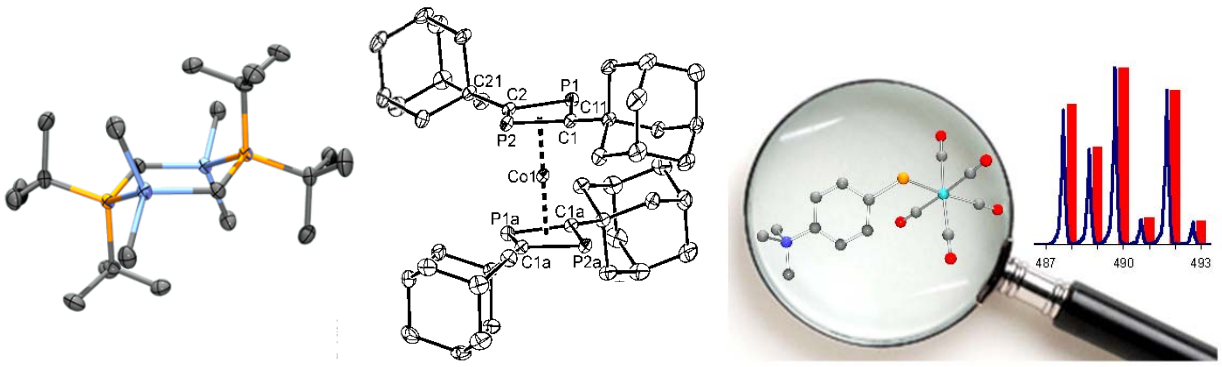


Figure. Left: X-ray crystal structure of an FLP dimer; Middle: X-ray crystal structure of $[Co(\eta^4\text{-}P_2C_2Ad_2)_2]^-$ complex; Right: Graphical display and MS spectrum of $[Me_3NC_6H_4\text{–}P{=}W(CO)_5]^+$

Key publications 2008-2011

- Appelt, C.; Westenberg, H.; Bertini, F.; Ehlers, A.W.; Slootweg, J.C.; Lammertsma, K.; Uhl, W.; Geminal phosphorus/aluminum-based frustrated Lewis pairs: C-H versus C≡C activation and CO_2 fixation, *Angew. Chem. Int. Ed.* **2011**, *50*, 3925-3928; *Angew. Chem.* **2011**, *123*, 4011-4014; (highlighted in *Nachtrichten aus der Chemie* **2012**, 60, 221-222).

- Lyaskovskyy, V.; Elders, N.; Ehlers, A.W.; Lutz, M.; Slootweg, J. C.; Lammertsma, K.; Remarkable metal-complexed phosphorus analogues of the cyclopropenyl-carbene–cyclobutadiene rearrangement, *J. Am. Chem. Soc.* **2011**, *133*, 9704-9707.

- Jansen, H.; Läng, F.B.; Slootweg, J.C.; Ehlers, A.W.; Lutz, M.; Lammertsma K.; Grützmacher, H.; Synthesis, structure and reactivity of [N,N-Dimethyl-BABAR-Phos]OTf, *Angew. Chem. Int. Ed.* **2010**, *49*, 5485-5488; Angew. Chem. **2010**, *122*, 5617-5620; (Highlighted in *Nachtrichten aus der Chemie* **2011**, *59*, 228).

- Aktas, H.; Slootweg, J.C.; Lammertsma, K.; Nucleophilic phosphinidene complexes – access and applicability, *Angew. Chem. Int. Ed.* **2010**, *49*, 2102-2113; *Angew. Chem. Int. Ed.* **2010**, 122, 2148-2159 (inside cover).

- Couzijn, E.P.A.; Slootweg, J.C.; Ehlers, A.W.; Lammertsma, K.; 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.*

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- Jansen, H.; Samuels, M.C.; Couzijn, E.P.A; Slootweg, J.C.; Ehlers, A.W.; Chen, P.; Lammertsma K.; A carbene-like phosphinidene complex caught in the act, *Chem. Eur. J.* **2010**, 16, 1454-1458 (front cover).

- Wolf, R.; Slootweg, J.C.; Ehlers, A.W.; Hartl, F.; De Bruin, B.; Lutz, M.; Spek, A.L.; Lammertsma, K.; A phosphorus analogue of bis(η4-cyclobutadiene)iron(0), *Angew. Chem. Int. Ed.* **2009**, *48*, 3104-3107; *Angew. Chem.* Int. Ed. **2009**, 121, 3150-3153 (front cover).

- Burck, S.; Van Assema, S.G.A.; Lastdrager, B.; Slootweg, J.C.; Ehlers, A.W.; Otero, J.M.; Dacunha-Marinho, B.; Llamas-Saiz, A.L.; Overhand, M.; Van Raaij, M.J.; Lammertsma, K.; Bis-phosphine-functionalized cyclic decapeptides based on the natural product gramicidin S: a potential scaffold for transition-metal coordination, *Chem. Eur. J.* **2009**, 15, 8134-8145 (frontispiece).

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, is rapidly being depleted. 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.

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) 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 2008-2011

- Elders, N.; Van der Born, D.; Hendrickx, L.J.D.; Timmer, B.J.J.; Krause, A.; Janssen, E.; De Kanter, F.J.J.; Ruijter, E.; Orru R.V.A.; The Efficient One-Pot Reaction of up to Eight Components by the Union of Multicomponent Reactions, *Angew. Chem. Int. Ed.* **2009**, *48* (32), 5856-5859.

- Znabet, A.; Ruijter, E.; De Kanter, F.J.J.; Kohler, V.; Helliwell, M.; Turner, N.J.; Orru, R.V.A.; Highly Stereoselective Synthesis of Substituted Prolyl Peptides Using a Combination of Biocatalytic Desymmetrization and Multicomponent Reactions, *Angew. Chem. Int. Ed.* **2010**, *49* (31), 5289-5292.

- Ruijter, E.; Scheffelaar, R.; Orru, R.V.A.; Multicomponent Reaction Design in the Quest for Molecular Complexity and Diversity, *Angew. Chem. Int. Ed.* **2011**, *50* (28), 6234-6246.

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.

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 analogues 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 unreactive 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 2008-2011

- Walvoort, M.; Lodder, G.; Mazurek, J.; Overkleeft, H.S.; Codée, J.D.C.; Van der Marel, G.A.; Equatorial anomeric triflates from mannuronic acid esters, *J. Am. Chem. Soc.* **2009**, *131*, 12080.

- Van der Heden van Noort, G.J.; Van der Horst, M.G.; Overkleeft, H.S.; Van der Marel G.A.; Filippov, D.V.; Synthesis of mono-ADP-ribosylated oligopeptides using ribosylated amino acid building blocks, *J. Am. Chem. Soc.* **2010**, *132*, 5236.

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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

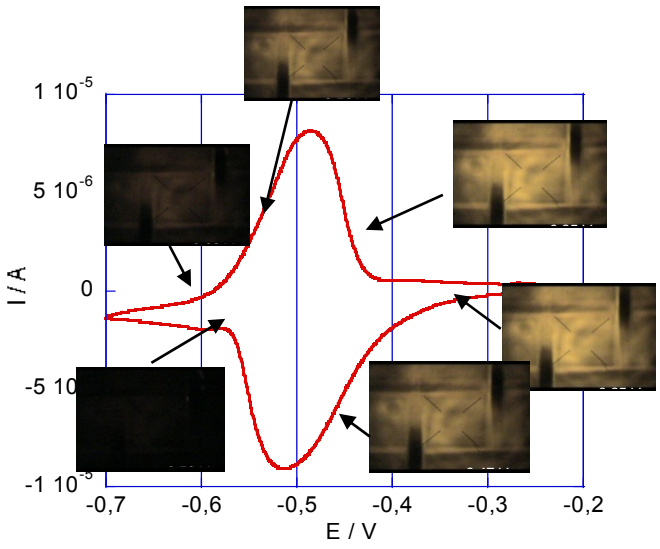
Prof. dr. J.N.H. Reek, Prof. dr. F. Hartl, Dr. B. de Bruin,
Dr. J.I. van der Vlugt (UvA)

Research topics

- Development of new approaches in transition metal catalysis and catalyst recovery, including supramolecular approach, ligand design, bioinspired approaches, 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.
- 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, relevant for photodriven reactions.
- Photo- and electrocatalytic activation of carbon dioxide and generation of molecular hydrogen.

Summary of research activities

We have developed several ligands for transition metal catalytic processes, including hybride bidentate ligands for asymmetric hydrogenation and asymmetric hydroformylation and new catalyst for polymerization reactions. Also, we have developed novel strategies for ligand selection rather than ligand screening protocols. A first example (Nature Chemistry 2010) was based on relative stability of the resting state of the reaction, identified by MS spectroscopy, whereas in a second example we have used co-factors to steer the selectivity of a reaction (JACS 2011). From competition experiments it was found that the strongest binder also gave the highest selectivity.
In addition to these successes we also further explored the development of encapsulated catalysts.



Reversible redox cycle of fluorescent p-chloromethoxytetrazine investigated with a thin-layer electrochemical cell coupled to an epifluorescence microscope in a total reflection fashion.

Photocatalytic formation of molecular hydrogen was further investigated with promising [Fe2S2]-linker-metal porphyrin triads featuring phosphoramidite bridges. The systems show improved photostability, performance and versatility compared with assemblies containing pyridylphosphine linkers.
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 α-diimine ligands, which does not require addition of sacrificial electron donors.

Key publications 2008-2011

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Future developments

We will continue to develop new innovative tools for transition metal catalytic processes. An important research line in Amsterdam is the development of catalyst for green energy applications, i.e. photodriven water splitting reaction to form hydrogen and oxygen. This is partly done in collaboration with Brouwer, and other groups in Netherlands that take part in the Biosolarcell program.

The NWO ECHO project *Light-Driven Dihydrogen Production in [2Fe2S]-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 metalloporhyrins 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).

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 used to produce phosphorylated compounds and carbohydrates at a gram scale. We also studied the enzymatic sulfation of quercitine (a natural flavinoid) using an arylsulfotransferase
In collaboration with the Department of Conservative and Preventive Dentistry, Academic Centre for Dentistry, Amsterdam the antimicrobial effect of the vanadium chloroperoxidase toward in vitro *E. faecalis* biofilms has been investigated and it is been concluded that the enzyme might provide an addition to current endodontic treatment, possibly as an antimicrobial dressing. In the cooperation with Prof. Dr. W. Tremel (Institut für Anorganische Chemie und Analytische Chemie, Johannes Gutenberg Universität, Mainz, Germany) the enzyme-like activities of the vanadium pentoxide nanoparticles have been further investigated and in particular the brominating activity in the presence of hydrogen peroxide.

Key publications 2008-2011

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Future developments

We continued our attempts 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. The successful cooperation with Prof. Dr. W. Tremel on the properties of the vanadium pentoxide nanoparticles will also be continued. The use of the arylsulfotransferase in the sulfation of a variety of compounds will be further investigated.

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, characterization of redox proteins, and depth analysis through nontransparent samples using time-resolved Raman spectroscopy.

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.

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.

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

Light-induced chemical conversions play a key role in many technological and biological processes. The research of the Molecular Photonics group addresses the key areas of *Dynamics of supramolecular and biomolecular systems*, *Photoprocesses in nanostructures*, and *Photochemical processes*. Highlights of our research activities in 2011 include the following.

Luminescent silicon. A study on the photophysical properties of small silicon nanoparticles in collaboration with Zuilhof (WUR) was completed. In addition to luminescence, a long-lived transient absorption signal was observed, which until now was never reported for silicon nanoparticles. Somewhat to our disappointment, the photochemical stability was insufficient for single particle luminescence observation, and the two-photon absorption cross section was small. Some of the results were quite different from those of other workers in the field with superficially similar materials. It is clear that improvement of the synthesis and purification methods is necessary for this field. Only when robust protocols are available that are reproducible in different laboratories, consistent results can be expected to emerge (*J. Phys. Chem. C* **2011**, *115*, 20888-20895).

Tripodal osmium polypyridyl complexes for self-assembly on platinum nanoparticles. The combination of platinum nanoparticles with a tripodal osmium complex that anchors to the metal surface leads, under visible light irradiation, to the formation of solvated electrons. The formation kinetics is limited by the detachment of the electron from the platinum surface into the solution, the particle showing a type of capacitor behavior (*J. Phys. Chem. Letters.* **2011**, *2*, 1460–1463).

Breakthrough in concentration quenching threshold of upconversion luminescence. Aiming at improving the upconversion luminescence efficiency of rare earth (RE) ions doped nanoparticles for medical application, a novel strategy of spatially separating the doping area has been adopted leading to an impressive increase of the quenching threshold from 2% to 8% (*Chem. Comm*. **2011**, *47*, 11957-11959).

Critical shell thickness for singlet oxygen generation in upconversion core/shell nanoplatform. The influence of the structure of upconversion nanoparticles on their Förster resonant energy transfer (FRET) applications has been studied using nano-

conjugates constructed by core/shell upconversion $NaYF_4:Yb^{3+},Er^{3+}@NaYF_4$ nanoparticles and photosensitizers. The optimal shell thickness for the most efficient FRET has been determined from the photophysics and singlet oxygen generation. It has been found that this optimal shell thickness is a trade-off between the opposing optimal conditions for upconversion and FRET efficiency (*J. Phys. Chem. Letters* **2011**, *2*, 2083-2088).

Cyclodextrin-based systems for photoinduced hydrogen evolution. Light-driven catalytic three component systems for the reduction of protons, consisting of a cyclodextrin-appended iridium complex as photosensitizer, a viologen-based electron relay, and cyclodextrin-modified platinum nanoparticles as the catalyst, were found to be capable of producing molecular hydrogen effectively in water, using a sacrificial electron donor. By investigating different photocatalytic systems, it was found that the amount of hydrogen produced was directly proportional to the emission quantum yield of the photosensitizer (*Phys. Chem. Chem. Phys.* **2011**, *13*, 7903-7909).

Solvatochromic rotaxanes. Fluorescent molecules of which absorption and emission colors depend on the medium have been a longstanding research topic in our laboratory. We now combined this functionality with molecular shuttles, leading to a strongly fluorescent bistable rotaxane in which the relative position of the macrocyclic ring with respect to the fluorophore gives a strong response in the spectral domain (*Chem. Comm.* **2011**, *47*, 4977-4979).

Ultrafast dynamics of a nanoscopic wheel probed by vibrational photon echoes. The dynamics of the hydrogen bonds connecting the axle and rim of a rotaxane-based nanometer-size wheel in solution have been investigated using femtosecond infrared photon echoes. We find that the hydrogen-bond dynamics is liquid-like on a time scale 1 ps and less, but structurally frozen on longer (up to at least 200 ps) time scales (*J. Chem. Phys.* **2011**, *134*, 134504/1-134504/7).

Switchable rotaxanes in the gas phase. The structural and dynamical properties of isolated, jet-cooled [2]rotaxanes that feature two binding stations incorporated into the thread have been studied using IR spectroscopy and *ab initio* calculations. Considering the size and structural as well as conformational complexity of such systems, this is quite a remarkable accomplishment. This analysis has elucidated the conformational structure of each component and has provided vibrational markers that enable one to map interactions between the various components. Equally important, the experiments form the basis for subsequent studies of shuttling in the gas phase (*J. Phys. Chem. A* **2011**, *115*, 9669-9675).

Electronic spectroscopy of ions in helium nanodroplets. Recently, we developed in collaboration with Drabbels (EPFL) a new experimental method to record IR spectra of molecular cations in helium droplets that has now been adopted to record electronic spectra of molecular ions. These experiments constitute the first application of helium nanodroplets to obtain electronic spectra of molecular ions. Since helium droplets can be readily doped directly with a variety of ions from different sources, the method is extremely versatile (*J. Phys. Chem. Letters.* **2011**, *2*, 1563–1566).

The electronic ground state of the naphthyl cation. Infrared spectroscopy of the isolated naphthyl carbocation provides evidence for a triplet electronic ground state, in which a π electron is promoted to the vacant σ orbital. Previous computational studies have been ambiguous as to the relative stabilities of the singlet and triplet states; DFT calculations predict both states to be practically isoenergetic (*Angew. Chem. Int. Ed.* **2011**, *50*, 7004-7007).

Key publications 2008-2011

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- Kluwer, A.M.; Kapre, R.; Hartl, F.; Lutz, M.; Spek, A.L.; Brouwer, A.M.; Van Leeuwen, P.W.M.N.; Reek, J.N.H.; Self-assembled biomimetic [2Fe2S]-hydrogenase-based photocatalyst for molecular hydrogen evolution, *Proc. Natl. Acad. Sci. USA* **2009**, *106,* 10460-10465.

- Marras, F.; Kluwer, A.M.; Siekierzycka, J.R.; Vozza, A.; Brouwer A.M.; Reek, J.N.H.; Phosphorus ligand imaging with two-Photon fluorescence spectroscopy: towards rational catalyst immobilization, *Angew. Chem. Int. Ed.* **2010**, *49*, 5480–5484.

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- De Boer, W.D.A.M.; 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 Nanotech.* **2010**, *5*, 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 and for understanding astrochemical phenomena. The strong collaborations with the Free Electron Laser facilities FELIX, FELICE, and FLARE will be continued and expanded.

The application of chiro-optical spectroscopic techniques such as 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. Extension to (Resonance) Raman Optical Activity is foreseen. 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.

Fluorescent probes are finding more and more applications, in polymer science and in the studies together with the Institute of Physics on colloidal matter. The combination of molecular probes and optical microscopy is still relatively under-developed in these fields. Fluorescence is also explored as a new tool in the study of organocatalysts.

Next to further theoretical development and practical application of the "Karplus relation for charge transfer interaction", focus will be directed at photo-induced processes (especially triplet charge recombination) in new materials for organic solar cells as well as the development and study of new photo-catalytic systems. Our long-standing experience in the field of photoinduced electron transfer is being exploited in a new project together with the Homogeneous Catalysis group aiming at the catalytic oxidation of water. Photosensitizers are under development for supramolecular light-harvesting and charge separating assemblies.

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.

The upconversion nanoplatform 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.

New photonic nano-labellers featured by cell/tissue labelling without excitation light are under development. This new generation of nanoplatforms are expected to have wide applications in biology and medicine including cell probing and image-guided surgery.

Biomolecular Analysis and Spectroscopy

Prof. dr. C. Gooijer (retired 1 June 2011), 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
- Pico-second time-gated Raman spectroscopy for analyzing nontransparant samples
- Optimization of Raman methods for (fossilized) bacteria on minerals for future Mars missions.
- High-resolution fluorescence spectroscopy under cryogenic conditions
- UV-resonance 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 (VENI project of Dr Diego Millo).

Time-resolved and steady state fluorescence methods were mainly concentrated on the antihistamines (inverse agonists) mepyramine and tripelennamine. 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 complex 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. Furthermore, the technique was successfully applied to detect concealed explosives behind several mm of non-transparent polymers.

Time-resolved fluorescence and phosphorescence was applied to study the enantioselective binding of chiral drugs to the transport protein human serum albumin. Static and dynamic process could be studied at the nanosecond timescale as well as the millisecond timescale.

In order to contribute to the development of new instrumentation for future planetary studies (e.g., Mars), a project was started on optimizing Raman characterization methods for (fossilized) bacteria on mineral backgrounds. Focus will be on the detection of biomarkers such as UV protective compounds in earth extremophiles.

Key publications 2008-2011

- Tardioli, S.; Buijs, J.B.; Gooijer, C.; Van der Zwan, G.; Structure elucidation of fluorescent H1 antihistamines by ultraviolet resonance Raman spectroscopy. Solvent structures of tripelenamine and mepyramine, *J. Raman Spectrosc.*, **2011**, *42*, 1016-1024.

- Petterson, I.E.I.; López, M.; Garciá-Ruiz, C.; Gooijer, C.; Buijs, J.B.; Ariese, F.; Noninvasive detection of concealed explosives: depth profiling through opaque plastics by time-resolved Raman spectroscopy, *Anal. Chem*. **2011**, *83*, 8517-8523.

- Lammers, I.; Buijs, J.; Van der Zwan, G.; Ariese, F.; Gooijer, C.; Phosphorescence for sensitive enantioselective detection in chiral capillary electrophoresis, *Anal. Chem.* **2009**, *81*, 6226-6233.

Future developments

Current research on heme proteins focusses on the immobilization of cytochrome P450BM3 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 C4,IDO, TDO) will be the topic of investigation. Present attention is on the spectroelectrochemical characterization of biofilms on electrode surfaces.

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, as well as the detection of traces of explosives under resonance Raman conditions at 244 nm.

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. Exploratory measurements with skin and artificial skin phantoms are very promising. Excitation is applied at 720 nm to reduce fluorescence as well as absorption losses by hemoglobine and other colored compounds. In addition, depth Raman using time-resolved detection is being used to look inside heterogeneous catalysts, and (Monte Carlo) simulations are applied to study the photon migration processes through nontransparent samples.

We will continue to work on the development of new Raman instrumentation for future Mars missions. Focus is on optimizing Raman characterization methods for (fossilized) bacteria on mineral backgrounds, and the detection of biomarkers such as UV protective compounds in earth extremophiles.

In collaboration with other groups at LaserLaB VU and with Philips, a PhD project will start on nanospectroscopy, a combination of AFM technology and molecular spectroscopic techniques such as Raman and fluorescence. The project is part of the nanonextNL initiative.

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 continues 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 2008-2011

- Mathies, G.; Blok, H.; Disselhorst, J.A.J.M.; Gast, P.; Van der Meer, H.; Miedema, D.M.; Almeida, R.M.; Moura, J.J.G.; Hagen, W.R.; Groenen, E.J.J.; Contonues-wave EPR at 275 GHz: Application to high-spin Fe3+ systems, *J. Magn. Reson.* **2011**, *210*, 126-132.

- Drescher, M.; Van Rooijen, B.D.; Veldhuis, G.; Subramaniam, V.; Huber, M.; A Stable Lipid-Induced Aggregate of α-synuclein, *J. Am. Chem. Soc.* **2010**, *132*, 4080-4082.

- Ruijgrok, P.V.; Verhart, N.R.; Zijlstra, P.; Tchebotareva, A.L.; Orrit, M.; Brownian fluctuations and heating of an optically aligned gold nanorod, Phys. Rev. Lett. **2011**, 107, 037401.

- Purchase, R.; Völker, S.; Spectral hole burning: examples from photosynthesis, *Photosynth. Res.* **2009**, *101*, 245-266.

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 developed further to study the dynamics and interactions of molecules and proteins, both in solutions and membrane related systems.

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. 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. 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:

The light-harvesting complex II (LHCII) is the main component of the antenna system of plants and green algae and plays a major role in the capture of sun light for photosynthesis. The LHCII complexes have also been proposed to play a key role in the optimization of photosynthetic efficiency through the process of state 1–state 2 transitions and are involved in down-regulation of photosynthesis under excess light by energy dissipation through non-photochemical quenching (NPQ). We presented the first solid-state magic-angle spinning (MAS) NMR data of the major light-harvesting complex (LHCII) of *Chlamydomonas reinhardtii*, a eukaryotic green alga. We are able to identify nuclear spin clusters of the protein and of its associated chlorophyll pigments in ^{13}C–^{13}C dipolar homonuclear correlation spectra on a uniformly ^{13}C-labeled sample. In particular, we were able to resolve several chlorophyll 13^1 carbon resonances that are sensitive to hydrogen bonding to the 13^1-keto carbonyl group. The data show that ^{13}C NMR signals of the pigments and protein sites are well resolved, thus paving the way to study possible structural reorganization processes involved in light-harvesting regulation through MAS solid-state NMR.

Phytochrome photoreceptors mediate light responses in plants and in many microorganisms. We have reported H-1-C-13 magic-angle spinning NMR spectroscopy of the sensor module of cyanobacterial phytochrome Cph1. Two isoforms of the red-light absorbing Pr ground state are identified. Conclusive evidence that photoisomerization occurs at the C15-methine bridge leading to a beta-facial disposition of the ring D is presented. In the far-red-light absorbing Pfr state, strong hydrogen-bonding interactions of the D-ring carbonyl group to Tyr-263 and of N24 to Asp-207 hold the chromophore in a tensed conformation. Signaling is triggered when Asp-207 is released from its salt

bridge to Arg-472, probably inducing conformational changes in the tongue region. A second signal route is initiated by partner swapping of the B-ring propionate between Arg-254 and Arg-222.

Quantum chemical modeling:
Recent experimental data point to an asymmetric ground-state electronic distribution in the special pair (P) of purple bacterial reaction centers, which acts as the primary electron donor in photosynthesis. We have performed a DFT investigation on an extended model including the bacteriochlorophyll dimer and a few relevant surrounding residues to explore the origin of this asymmetry. We find strong evidence that the ground-state electron density in P is intrinsically asymmetric due to protein-induced distortions of the porphyrin rings. Moreover, the electron charge asymmetry is strongly modulated by the specific orientation of the $C3^1$ acetyl group, which is hydrogen bonded to His168. The electronic excitation has a significant charge transfer character inducing a displacement of electron charge from P_L to P_M, in agreement with experimental data in the excited state. These results are relevant for the understanding of the unidirectional electron transfer path in photosynthesis.

Key publications 2008-2011

- 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**, *106-21*, 8525-8530.

- Wawrzyniak, P.K.; Beerepoot, M.T.; De Groot, H.J.; Buda, F., Acetyl group orientation modulates the electronic ground-state asymmetry of the special pair in purple bacterial reaction centers. *Phys. Chem. Chem. Phys* **2011,** *13*, 10270.

- Song, C.; Psakis, G.; Lang, C.; Mailliet, J.; Gartner, W.; Hughes, J.; Matysik, J., Two ground state isoforms and a chromophore D-ring photoflip triggering extensive intramolecular changes in a canonical phytochrome, *Proc. Natl. Acad. Sci. USA* **2011,** *108*, 3842.

- De Groot, H.J.M.; Chapter 28: Engineered Natural Photosynthesis, in: Fundamentals of Materials for Energy and Environmental Sustainability, edited by Dave Ginley and David Cahen, published by Cambridge University Press, **2011**

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 mechanisms. We will focus on the mechanisms of charge separation and 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.

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 multichannel ionic fragmentation dynamics in CF_3I was studied by femtosecond pulse shaping and velocity map photoelectron photoion coincidence imaging. In this first study we focussed on the influence of LCD-shaped laser pulses on the molecular dynamics. The three-dimensional recoil distribution of electrons and ions were imaged in coincidence using a single time-of-flight delay line detector. By fast switching of the voltages on the various velocity map ion lenses after detection of the electron, both the electron and the coincident ion are measured with the same imaging detector. These results demonstrate that a significant simplification of a photoelectron-photoion coincidence imaging apparatus is in principle possible using switched lens voltages. It is observed that shaped laser fields like chirped pulses, double pulses, and multiple pulses can enhance the CF_3^+/CF_3I^+ ratio by up to 100%. We propose that the control mechanism is determined by dynamics on neutral excited states and we discuss the results in relation to the location of electronically excited (Rydberg) states of CF_3I.

In another study we reported slice imaging polarization experiments on the state-to-state photodissociation at 42 594 cm^{-1} of spatially oriented OCS(v_2 = 1|JlM = 111) - CO(J) + S($^1D_2$). Slice images were measured of the three-dimensional recoil distribution of the S($^1D_2$) photofragment for different polarization geometries of the photolysis and probe laser. The high resolution slice images show well separated velocity rings in the S($^1D_2$) velocity distribution. The velocity rings of the S($^1D_2$) photofragment correlate with individual rotational states of the CO(J) cofragment in the J_{CO} = 57–65 region. The angular distribution of the S($^1D_2$) velocity rings are extracted and analyzed using two different polarization models. The first model assumes the nonaxial dynamics evolves after excitation to a single potential energy surface of an oriented OCS(v2 = 1|JlM = 111) molecule. The second model assumes the excitation is to two potential energy surfaces, and the OCS molecule is randomly oriented. In the high J region (J_{CO} = 62–65) it appears that both models fit the polarization very well, in the region J_{CO} = 57–61 both models seem to fit the data less well. From the molecular frame alignment moments the m-state distribution of S($^1D_2$) is calculated as a function of the CO(J) channel. A comparison is made with the theoretical m-state distribution calculated from the long-

range electrostatic dipole–dipole plus quadrupole interaction model. The $S(^1D_2)$ photofragment velocity distribution shows a very pronounced strong peak for $S(^1D_2)$ fragments born in coincidence with CO(J = 61).

Key publications 2008-2011

- Vredenborg, A.; Roeterdink, W.G.; Janssen, M.H.M.; A photoelectron-photoion coincidence imaging apparatus for femtosecond time-resolved molecular dynamics with electron TOF resolution of σ=18 ps and energy resolution ΔE/E=3.5%, *Rev. Sci. Instrum.* **2008**, *79*, 063108.

- Lipciuc, M. L.; Rakitzis, T.P.; Meerts, W.L.; Groenenboom, G.C.; Janssen, M.H.M.; Towards the complete experiment: Measurement of S(1D2) polarization in correlation with single rotational states of CO(J) from the photodissociation of oriented OCS(v2=1|JlM=111), *Phys. Chem. Chem. Phys.* **2011**, *13*, 8549.

- Irimia, D.; Janssen, M.H.M.; Toward elucidating the mechanism of femtosecond pulse shaping control in photodynamics of molecules by velocity map photoelectron and ion imaging, *J. Chem. Phys*. **2010**, *132*, 234302.

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 have developed a novel technique for the detection of chiral molecules using photoelectron circular dichroism. Employing femtosecond multi-photon ionization in combination with photoelectron-photoion coincidence imaging we have demonstrated a high sensitivity for the detection of mass-selected chiral molecules. 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. The piezo valve has presently been purchased by some 15 laboratories worldwide.

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-uhv 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 2008-2011

- Rodríguez, P.; Kwon,Y.; Koper, M.T.M.; The promoting effect of adsorbed carbon monoxide on the oxidation of alcohols on a gold catalyst, *Nature Chem.* **2012**, *4*, 177-182.

- Yanson, A.I.; Rodriguez, P.; Garcia-Araez, N.; Mom, R.V.; Tichelaar, F.D.; Koper, M.T.M.; Cathodic corrosion: a quick, clean and versatile method for the synthesis of metallic nanoparticles, *Angew. Chem. Int. Ed.* **2011**, *50*, 6346-6350.

- Van der Niet, M.J.T.C.; Den Dunnen, A.; Koper, M.T.M.; Juurlink, L.B.F.; Tuning hydrophobicity of platinum by small changes in substrate morphology, *Phys. Rev. Lett.* **2011**, *107*, 146104 (1-4).

- Van der Niet, M.J.T.C.; Den Dunnen, A.; Juurlink, L.B.F.; Koper, M.T.M.; Co-adsorption of O and H_2O on nano-structured platinum surfaces: does OH form at steps?, *Angew. Chem. Int. Ed.* **2010**, *49*, 6572-6575.

- Duca, M.; Oroval Cucurella, M.; Rodriguez, P.; Koper, M.T.M.; Direct reduction of nitrite to N_2 on a Pt(100) electrode in alkaline media, *J. Am. Chem. Soc.* **2010**, *132*, 18042-18044.

Future developments

The group will continue to strengthen its position on electrochemical and ultra-high-vacuum surface science and in particular in the combination of both. Future developments will include a more visible role of theoretical and computational chemistry, and the deployment of in situ scanning probe methods, such as scanning tunneling microscopy (STM) in collaboration with the group of Frenken at the Leiden Institute of Physics.

Raymond and Beverly Sackler Laboratory for Astrophysics

Prof. dr. H. Linnartz (UL)

Research topics

- IR and UV/VIS spectroscopy
- Solid state astrochemistry
- Molecular transients of astrophysical interest
- Plasma expansions

Summary of research activities

The space around and between stars is highly dilute. Despite the low temperatures and high radiation fields, an intriguing mixture of small and complex, stable and reactive species has been identified in the ISM, the interstellar medium. 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 program focuses on this interplay, by providing spectral fingerprints of molecular transients of astrophysical interest and studying the solid state processes at work that provide pathways towards molecular complexity in space.

In 2011 a new setup has been constructed in which broad band cavity enhanced spectroscopy is combined with supersonic planar plasma expansions to search for carbon chain radicals of interstellar interest. This setup is meanwhile fully operational. See also www.laboratory-astrophysics.eu. Another research project 'Shining light on ice' was initiated within the Dutch Astrochemistry Program, in which collaborations exist also within the HRSMC.

On March 18th, Nadine Wehres defended her thesis on 'Optical spectroscopy of interstellar and circumstellar molecules; a combined laboratory and observational study' (promotores Tielens/Linnartz). On November 4th, Sergio Ioppolo (promotores Linnartz/van Dishoeck) obtained the Dick Stufkens Award for his thesis on 'Surface Formation Routes of Interstellar Molecules' in which the formation of small molecules –water, carbon dioxide and methanol – was explained upon hydrogenation reactions of interstellar ice analogues. Dr. Wehres continued her career with a postdoc position at the University of Boulder, Dr. Ioppolo obtained an Marie Curie OEF grant and started a postdoc position at Caltech.

In 2011 a major breakthrough was obtained in characterizing photo-induced ice desorption mechanisms, in wavelength dependent experiments using the VUV beamline DESIRS at the synchrotron facility SOLEIL in France. See key publications.

Key publications 2008-2011

- Ioppolo, S.; Cuppen, H.M.; Romanzin, C.; van Dishoeck, E.F.; Linnartz, H.; Laboratory evidence for efficient water formation in interstellar ices; *Astrophys. J. Lett.* **2008**, 686, 1474.

- Öberg, K.I.; Garrod, R.T.; Van Dishoeck, E.F.; Linnartz, H.; Formation rates of complex organics in UV irradiated CH_3OH-rich ices I: Experiments, *Astron. Astrophys.* **2009**, *504*, 891.

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- Fayolle, E.C.; Bertin, M.; Romanzin, C.; Michaut, X.; Öberg, K.I.; Linnartz, H.; Fillion, J.H.; CO ice photodesorption – a wavelength dependent study; *Astrophys. J. Lett.*, **2011**, *735*, L36.

Future developments

In collaboration with Spinoza winners Tielens and van Dishoeck laboratory projects are initiated to study the photo-induced behavior of molecules of interstellar interest.

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 **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. Extensions of subsystem DFT methods for charge-transfer processes are explored. 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.

Theoretical Chemistry

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

Research topics

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

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 density matrix theory and computational methods derived from these theories are central themes, 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 2008-2011

- Wassenaar, J.; Jansen, E.; van Zeist, W.-J.; Bickelhaupt, F.M.; Siegler, M.A.; Spek, A.L.; Reek, J.N.H.; Catalyst Selection based on Intermediate Stability measured by Mass Spectrometry, *Nature Chem.* **2010**, *2*, 417-421.

- Pierrefixe, S.C.A.H.; Van Stralen, S.J.M.; Van Stralen, J.N.P.; Fonseca Guerra, C.; Bickelhaupt, F.M.; Hypervalent Carbon. "Freezing" the SN2 Transition State, *Angew.Chem.* **2009**, *121*, 6591-6593; *Angew. Chem. Int. Ed.* **2009**, *48* 6469-6471.

- Van der Wijst, T.; Fonseca Guerra, C.; Swart, M.; Bickelhaupt, F.M.; Lippert, B.; A Ditopic Ion-Pair Receptor Based on Stacked Nucleobase Quartets, *Angew.Chem.* **2009**, *121*, 3335-3337; *Angew. Chem. Int. Ed.* **2009**, *48*, 3285-3287.

- Jacob, C.R.; Beyhan, S.M.; Bulo, R.E.; Gomes, A.S.P.; Götz, A.W.; Kiewisch, K.; Sikkema, J.; Visscher, L.; PyADF — A scripting framework for multiscale quantum chemistry, *J. Comp. Chem.* **2011**, *32*, 2328.

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- Jacob, C.R.; Visscher, L.; A subsystem density-functional theory approach for the quantum chemical treatment of proteins, *J. Chem. Phys.* **2008**, *128*, 155102.

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- Bernasconi, L.; Belanzoni, P.; Baerends E.J.; An abiotic analogue of the diiron(IV)oxo 'diamond core' of soluble methane monooxygenase generated by direct activation of O_2 in aqueous Fe(II) / EDTA solutions: thermodynamics and electronic structure, *Phys. Chem. Chem. Phys.* **2011**, *13*, 15272-15282.

- Nicu, V.P; Baerends, E.J.; Robust normal modes in vibrational circular dichroïsm spectra, *Phys. Chem. Chem. Phys*. **2009**, *11*, 6107-6118.

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 investigated. Use of O_2 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.

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 telomere 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).

Computational Chemistry

Prof. P.G. Bolhuis, Prof. Dr. E.J. Meijer, Dr. B. Ensing, Dr. D. Dubbeldam, Dr. J. Vreede (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. Below highlights of the progress made in 2011 are listed.

Protein conformational changes (Bolhuis, Vreede, Ensing)

In proteins and enzymes, the local environment of an active cofactor plays an important role in controlling the outcome of a functional reaction. The Photoactive Yellow Protein (PYP) is a prime example of signaling protein, sensitive to light. We revealed key aspects of the signaling mechanism of PYP. 1) In a combined experimental and simulation study we addressed the effect of substituting proline-68, positioned near, but not in direct contact with the chromophore, with other neutral amino acids. Our study revealed that the hydrogen bond interactions around the chromophore and the access of water molecules in the active site of the protein determine the efficiency of photoisomerization. The mutants provide additional hydrogen bonds to the chromophore, directly and by allowing more water molecules access to its binding pocket. (van Stokkum, Vreede and co-workers, J. Phys. Chem. B 115, 6668, 2011).

2) In separate studies we addressed the chemical and conformational changes in the PYP photocycle. The of the initial proton-transfer reaction in the chromophore binding pocket was revealed using transition path sampling simulations in combination with a hybrid quantum/force-field (QM/MM) level of theory. We discovered that the proton donation from Glu46 to the chromophore is concerted with a restructuring of the hydrogen-bond network involving various neighboring residues (Tyr42, Arg52 and Thr50) order to stabilize the negative charge on Glu46. The subsequent protein unfolding was addressed using the in-house developed path-metadynamics method. This provided the free energy profile along average transition pathway that involves a complex rearrangement of the chromophore binding pocket and its surrounding. (Vreede, Ensing, Meijer, Bolhuis, manuscripts in preparation).

Signal transduction upon binding of a ligand to a membrane protein can occur not only via allosteric conformational changes but also through fluctuations. We performed a numerical study on the influence of conformational fluctuations on the cooperativity of a binding reaction in a simple model of an integral membrane receptor consisting of transmembrane helices (Bolhuis and co-workers, Phys. Rev. Lett. 106, 168103 (2011)). We found that small fluctuations lateral as well as perpendicular to the membrane can increase the cooperativity, with the former more dominant. Moreover, too much fluctuation induces negative cooperativity. Proteins with fewer than four helices do not show positive cooperativity under any circumstances. This behavior is rather robust, and independent of the receptor topology or ligand size. Fluctuations measured in all-atom molecular dynamics simulations of a G-protein coupled receptor fall within the predicted region of maximum cooperativity.

Biomaterials (Bolhuis)

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. Previously, by extensive replica exchange molecular dynamics simulation we predicted the thermodynamically stable conformation of the middle block to be a ß-roll. Since the exact mechanism of the fibril formation remains unclear, we employed a multiscale modelling approach in combination with rare event simulations to elucidate key processes (Bolhuis and co-workers, Phys. Chem. Chem. Phys. 13, 10457, 2011.). Atomistic scale simulations on the silk-based block suggest a mechanism in which a polypeptide prefolded into a beta-roll structure docks to the growing end of a fibril through the formation of Glu-Glu sidechain contacts. Subsequently it can slide to the optimal position before water is expelled to form a dry interface between the fibril end and the attaching block copolymer. In addition, we find that the folded state of the silk-based block is further stabilised through interactions with its neighboring block. Templated folding may also play a role in case a partially folded polypeptide attaches. The coarse-grained simulations indicate that the attachment and subsequent sliding is mediated by the hydrophilic flanks in a size dependent manner. The hydrophilic blocks prevent random aggregation and allow growth only at the end of the fibril. Our multiscale approach may be used for other fibril-forming peptides.

Whey proteins such as β-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. β-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.

Chemical reactivity in complex environment (Ensing, Meijer)

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. In a recent studies, we addressed the hydration of metal cations and their role in the acid chemistry of confined

waters in interlayer space of smectites. In the latter study we also focussed owe also focused on the role of the smectite layer charge densities. Our study revealed that the layer charge enhances the water acidity enhancement in smectites, and that clear that clay frameworks can also enhance acidities of the cation-bound waters. As highly acidic cations (e.g. Mg^{2+}, Ca^{2+}, Al^{3+}, Fe^{3+}) occur as counterions in nature, their presence eventually makes the interlayer region a chemical environment of high acid activity. (Meijer and co-workers, Geochimica et Cosmochimica Acta 75, 4978, 2011).

Hard Materials (Dubbeldam, Meijer)

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.

MOFs: Recent experiments showed that synthesized chiral MOFs with the catalyst incorporated into the framework yields enhanced stability and separation in chiral epoxidation. To elucidate this phenomena we performed hybrid quantum-force field (QM/MM) simulations where we focused on the role of steric effects of the MOF on the enantioselectivity of (salen)Mn (Dubbeldam and co-workers, J. Mol. Catal. A: Chem. 334, 89, 2011). This study provided novel insight in 1) the most likely reaction pathway, 2) the difference between the pathway of the free molecular analogue and the one where the catalyst is incorporated into the framework and 3) the origin of the experimentally found improved stability and separation efficiency.

MOFs and zeolitic imidazolate frameworks (ZIFs) offer considerable potential for separating a variety of mixtures such as those relevant for CO(2) capture. In view of the vast number of MOFs, and ZIFs that have been synthesized there is a need for a systematic screening of potential candidates for any given separation task. A variety of metrics that quantify the separation performance, such as adsorption selectivity, working capacity, diffusion selectivity, and membrane permeability, are determined from a combination of Configurational-Bias Monte Carlo (CBMC) and Molecular Dynamics (MD) simulations. The practical utility of the suggested screening methodology is demonstrated by comparison with available experimental data. (Krishna and co-worker, PCCP, 13, 10593, 2011).

Carbon: The thermodynamic properties of graphite under extreme conditions of temperature and pressure are of fundamental interest for different fields, from geology to crystal growth, but very difficult to access experimentally. We have shown determined equation of state and thermoelastic properties of graphite in the pressure-temperature range that has been unexplored by experiments. These results will be important in the design and understanding of graphite-based strong materials. (Meijer, Fasolino and co-workers, Carbon 49, 364, 2011).

Soft Materials (Bolhuis)

We studied the mechanism of the homogeneous crystal nucleation from the supercooled liquid to the crystal phase in the soft-core colloid model for colloidal suspensions with the aim to identify optimal reaction coordinates (Bolhuis and co-workers, Phys. Rev. Lett. 106, 085701 2011, J. Chem.. Phys. 135, 154110 2011).

We select optimal reaction coordinates from a set of novel order parameters based on the local structure within the nucleus, by employing transition path sampling techniques combined with a likelihood maximization of the committor function. We found that nucleation is governed by solid clusters that consist of an hcp core embedded within a cloud of surface particles that are highly correlated with their nearest neighbors but not ordered in a high-symmetry crystal structure. We found that the size of the cloud of prestructured particles surrounding the crystalline nucleus enhances the description of the transition.
The results shed new light on the interpretation of the surface and volume terms in classical nucleation theory. Further, we showed that the rearrangement of the inner core of the nucleus according to Ostwald's step rule is a separate process, independent of the growth of the nucleus.

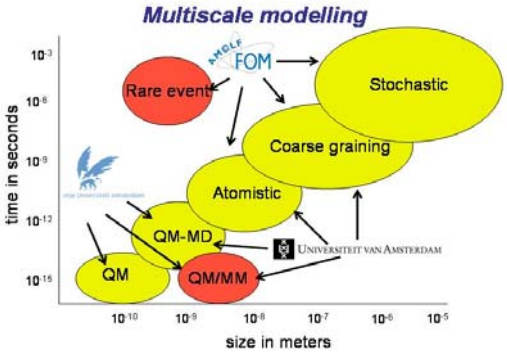
Methods for Simulating Complex Systems
The transition path sampling method is potentially very powerful to investigate conformational changes in proteins. However, the proteins can adopt multiple states, whereas conventional path sampling focuses only on two states.
We implemented and applied the multiple state version of transition path (interface) sampling for a model biomolecular system: alanine dipeptide in explicit water (Bolhuis and co-workers, J. Chem.. Phys. 135, 145102 2011). We extract the rate constant matrix for configurational changes between each pair of metastable states. The results are comparable with values from previous literature and show that the method is applicable to biomolecular systems.

In addition we elaborated on the properties of the reweighted path ensemble (Bolhuis and co-workers, J. Stat. Phys. 145, 841, 2011)). In this paper we derive several distribution functions for the recently introduced reweighted path ensemble: the configurational and path densities, the reactive current, and the generalized committors for the different path types. We relate these distributions to the free energy and to the expressions for the rate constant in the transition state theory, the reactive flux method, the transition path (interface) sampling framework, and the Bayesian path statistics. In addition, we compute the transmission coefficient (distribution) from the reweighted path ensemble. Finally, we derive the path sampling shooting point distributions. For a simple two dimensional Langevin model we illustrate how these novel distributions can be used as analysis tools in rare event simulations.

Key publications 2008-2011

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

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. A recent extension of the subsystem DFT method concerns its use as an effective diabatization scheme for charge-transfer processes.

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.

Key publications 2008-2011

- Neugebauer J.; Photophysical Properties of Natural Light-Harvesting Complexes Studied by Subsystem Density-Functional Theory, *J. Phys. Chem. B* **2008** *112*, 2207.

- Neugebauer J.; Subsystem-Based Theoretical Spectroscopy of Biomolecules and Biomolecular Assemblies, *ChemPhysChem* **2009**, *10*, 3148.

- Kovyrshin, A.; Neugebauer, J.; State-Selective Optimization of Local Excited Electronic States in Extended Systems, *J. Chem. Phys*. **2010**, *133*, 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

Research topic	Co-operating groups	Theme	University
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 fluoresence of flavonoids	Visscher - Ariese	2,3	VU
Calculations on homogeneous catalytic mechanisms	Ehlers - Bouwman	1	UvA, UL
Calculations on Multicomponent Syntheses	Bickelhaupt - Orru	1,3	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 - v.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 phosphinidine 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-orented rational design of catalysis	Bickelhaupt - Reek	1,3	VU, UvA
Glass transition (single-molecule probing)	Orrit - Brouwer	2	VU, UvA
Homogeneous catalysis by metal centers on organometallic complexes	Baerends - Reedijk	1,3	UL, VU

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
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 - v.Maarseveen	1	UvA
Photocatalysis	Brouwer - Reek - Hartl - v.d.Vlugt	1,2	UvA
Photocatalysis	Reek - v.d.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 pyridine N-oxides	Ariese - Gooijer - v.d.Zwan - Buma - Zhang	2	VU, UvA
Photoprocessing (dissociation,		2,3	VU, UL
Photosynthesis	De Groot - Koper	2,3	UL
Protons in aqueous environment	Meijer – Ensing - Woutersen	2,3	UvA
Resonance Raman spectroscopy of spheroidene	Van Hemert - Neugebauer	3	UL
Selective enzymatic phosphorylation	Hiemstra - Wever	1	UvA
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 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 - v.d.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 - v.Maarseveen	1	UvA, UL
Vibrational circular dichroism	Woutersen - De Bruin	1,2	UvA
Vibrational circular dichroism: applications and theory	Buma - Baerends	1,3	UvA, VU

Cooperations HRSMC-Cooperating groups Westfälische Wilhelms Universität Münster

Research topic	**Cooperating groups HRSMC (UvA, VU, UL)**	**Theme**	**Cooperating groups WWU Münster**
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	De Bruin	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
Phosphor activation	Lammertsma	1	Weigand
FLP	Lammertsma	1	Uhl
Phosphor sandwiches	Lammertsma	1	Wolf
Photophysics of coordination compounds: energy and electron transfer in supramolecular systems	Hartl - 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

2.5 Memberships and awards

Memberships organising committees international meetings 2011

Name staff member	Activity
Baerends	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
Bruin, de	Member Organizing Committee of the International Conference on Phosphorus Chemistry (ICPC 2012)
Buda	Member of Organising Committee, Lorentz workshop "Modeling Natural and Artificial Photosynthesis", March 2011, Leiden, The Netherlands
Ehlers	Member Organizing Committee of the International Conference on Phosphorus Chemistry 2012 (ICPC 2012)
Elsevier	Board EUCHEMS conferences Organometallic Chemistry since 2007Member
Ensing	Organizer Winter School for Theoretical Chemistry and Spectroscopy, Han sur Lesse, 2012.
Gooijer	Scientific Committee XIV Int. Symp. on Luminescence Spectrometry. Prague (Cz) July 2010
Groot, de	Member of Organising Committee, 8th European Biophysics Congress of European Biophysical Societies Association Solarfueltandem Network Meeting Mülheim
Hartl	COST program on catalysis for green energy
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 2012 (ICPC 2012)
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
Matysik	Spin-Chemistry Meeting 2011
Meijer	Coordinating organizer international school ´Understanding

	Molecular Simulation' 2010
Meijer	Member organizing committee ICTAC-14, Vlissingen (NL), 2012
Orrit	HBSM 2012, Tübingen, 27-31 August 2012
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
Slootweg	Member Organizing Committee of the International Conference on Phosphorus Chemistry 2012 (ICPC 2012)
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
Timmerman	Member of Scientific Advisory Board TIDES-meeting, Oligonucleotide & Peptide Research, Technology & Product Development
Vlugt, v.d.	Member Organizing Committee of the International Conference on Phosphorus Chemistry (ICPC 2012)
Visscher	Member Scientific Committee Relativistic Effects in Heavy Elements, (REHE2010), Beijing September 2010
Visscher	Organizer CECAM workshop on Modeling Natural and Artificial Photosynthesis, Lorentz Center

Board memberships scientific organisations/academies/awards

Name staff member	Activity
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 NWO
Bickelhaupt	Member TOP/ECHO committee NWO
Bickelhaupt	NWO Astrochemistry program committee
Bolhuis	Member FOM BRM programme committee
Bouwman	Board Member Leids Universiteits Fonds (LUF)
Bouwman	Member ACTS TA-committee Low Energy Routes
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 (2008-)
Buma	Chairman John van Geuns Fonds Foundation
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
Ensing	Member Educational Board HRSMC
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
Groot, de	Board member ESF EuroSolarFuel programme
Groot, de	Rapporteur to the European Science Foundation during scientific committee meeting in Bielefeld
Hartl	Visiting professorship at the Chuo University, Tokio (Japan)
Hartl	Visiting professorship at the Joseph Fourier University, Grenoble (France)
Hiemstra	Member of the International Advisory Board of the Organic Division of the Czech Chemical Society
Hiemstra	Member of the management committee of EU-COST action CM0905 ORCA "Organocatalysis"
Ingemann	Programme Director bachelor Scheikunde, UvA
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
Koper	Vice-President of the International Society of Electrochemistry
Koper	Board Member HRSMC
Koper	Board Member NIOK (Netherlands Institute for Catalysis Research)
Koper	Visiting Professor, Catalysis Reseach Center, Hokkaido University, Sapporo, Japan
Lammertsma	Chairman Organic Chemistry Section of the Royal Durch 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 Astrochemical Surface Science in Europe'
Linnartz	Solid state coordinator NWO Astrochemistry program committee
Linnartz	Board Member European Task Force Laboratory Astrophysics
Linnartz	External advisor Astrophysical Chemistry Group of the RSC / RAS
Maarseveen, van	Member of the management committee of EU-COST action CM0905 ORCA "Organocatalysis"
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 Review panels for NOW, AERES, DPG, FWO 2011
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 Durch Chemical Society (KNCV)
Orru	Chairman Organic Chemistry Section of the Royal Durch Chemical Society (KNCV)
Reedijk	Fellow of the Royal Society of Chemistry
Reedijk	Member Academia Europaea
Reedijk	Member board HRSMC
Reedijk	Member National Finnish Academy of Sciences
Reedijk	Member Royal Netherlands Academy of Arts and Sciences (KNAW)
Reek	Member of the management team of the biosolarcel (since 2010)
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	Director Amsterdam Center for Multiscale Modeling
Visscher	Dutch node director, CECAM
Visscher	Member werkgroep Supercomputers, NWO/NCF
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

Memberships international editorial boards 2011

Name staff member	Member of
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 Phyiscs
Bickelhaupt	ChemistryOpen
Bouwman	Applied Organometallic Chemistry (advisory board)
Bouwman	European Journal of Inorganic Chemistry (advisory board)
Brouwer	International Journal of Spectroscopy
Bruin, de	European Journal of Inorganic Chemistry
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)
Hemert, van	European Journal of Organic Chemistry (Editorial Board)
Hiemstra	European Journal of Organic Chemistry (Editorial Board)
Hiemstra	Progress in Heterocyclic Chemistry (Editorial Advisory Board)
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 -Physica Scripta
Matysik	Applied Magnetic Resonance
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, ChemBioChem (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
Reedijk	Journal of Inorganic Biochemistry
Reedijk	Polyhedron
Reek	European Journal of Inorganic Chemistry and ChemPlusChem
Stolte	Laser Chemistry (editorial advisor)
Timmerman	Review Editorial Board of Frontiers in Immunotherapies and Vaccines
Völker	Journal of Luminescence
Verhoeven	ChemPhysChem
Verhoeven	European Journal of Organic Chemistry
Verhoeven	International Journal of Photoenergy
Visscher	
Wever	
Williams	The Open Inorganic Chemistry Journal
Zhang	Guest editor Jounal of Luminescence

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.

Activities of 2011:

- The two weeks HRSMC Course '*Molecular Simulation*', organised under the auspices of CECAM (January 3-14 2011, UvA).
- The HRSMC Course '*Physical Methods in Inorganic Chemistry*' (Jan. 24, 28, 31 and Feb. 1, UvA/UL).

In addition to these Courses, the following special activities were organized:

- 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*'.
- Following the advice of the Education Committee, the first HRSMC lab visit within Research Theme 2 (Photochemistry and (Laser) Spectroscopy) was organized at the UL on January 25. Four HRSMC research groups (1) Biophysical Organic Structure, 2) Catalysis and Surface Chemistry, 3) Molecular Nano-Optics and Spins and 4) Astrophysics and Astrochemistry) were visited by PhD students, postdocs and staff members from other UL, VU and UvA HRSMC groups
  As within research theme 2 a lot of specialized equipment is used, this lab visits were organized to share expertise and knowledge, and to stimulate collaboration. The next lab visit will take place at the UvA/VU in 2013.
- Following the advice of the PhD platform, an Introduction Event for first-year PhD students as well as a Social Event for all HRSMC members was organized on June 9. At the Introduction Event several Board members and members of the Education Committee gave an overview of the research and educational activities within the HRSMC. The Social Event, a soccer tournament and some games, was organized by PhD students and the HRSMC, as a networking activity between UvA, UL and VU PhD students.

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

HRSMC Course *'Understanding Molecular Simulation'*, Molsim 2011
(January 3-14 2011, UvA)

Coordinators:	Dr. B. Ensing (UvA), Dr. E.J. Meijer (UvA) en I. Weijer (HRSMC)
Lecturers:	Prof. dr. P.Bolhuis (UvA), Dr. E.J. Meijer (UvA)
Guest Lecturers:	Dr. S. Abeln (VU), Prof. dr. D. Frenkel (AMOLF), Dr. C.P. Lowe (UvA), Prof. dr. B. Smit, (University of California, Berkeley), Prof. dr. T.H.J. Vlugt (TU Delft)
Participants:	89 (about 25% Master students and about 80 foreign participants)

HRSMC Course *'Physical Methods in Inorganic Chemistry'*
(January 24, 28, 31 and February 1, UvA/UL)

Coordinators:	Dr. S. Bonnet, Prof. dr. E. Bouwman, Dr. B. de Bruin, Prof. dr. C.J. Elsevier, I. Weijer (HRSMC), drs H.E. Zwaan-van der Plas (HRSMC)
Lecturers:	Dr. S. Bonnet, Prof. dr. E. Bouwman, Dr. B. de Bruin, Prof. dr. C.J. Elsevier, Dr. W. Fu, Prof. dr. F. Hartl, Dr. S. Ingemann Jørgensen and Dr. R. Williams
Guest Lecturers:	Dr. H. Kooijman and a Reaxys demonstration by Dr. B. Furter
Participants:	19 (4 Master students, 14 PhD en 1 postdoc, 9 UvA en 10 UL)

3.2 Symposium

The symposium, which was attended by ca. 140 scientists, also included poster sessions with 45 posters, mainly presented by PhD students. The format of last year symposium was also used for this symposium: less posters (about three posters per group selected by the work group leaders) and less posters per session, and more and shorter lectures.

The following lectures were given:
Theme 1 'Synthesis, Characterisation, Reactivity and Properties of Molecules'

- Dr. Eelco Ruijter (VU)
  "New tricks for (smelly) old dogs: exploiting atypical reactivity of isocyanides"
- PhD lecture of Sipeng Zheng (UL, group of Prof. dr. Lies Bouwman)
  "From molecules to materials: tuning the transition temperature and cooperativity of bapbpy-based mononuclear spin-crossover compounds"
- PhD lecture Pawel Dydio (UvA, group of Prof. dr. Joost Reek)
  "Supramolecular control of selectivity in transition metal catalysis using ligand functionalized with Anion Binding Pockets"

Theme 2 'Photochemistry and (Laser) Spectroscopy'

- Prof. dr. Fred Brouwer (UvA)
  "Looking into materials with fluorescence microscopy"
- Postdoc lecture of Dr. Bhargava Ram Niraghatam (VU, group of Prof. dr. Maurice Janssen)
  "A femtosecond mass-resolved microscope for chiral molecules"
- Postdoc lecture of Peter Zijlstra (UL, group of Prof. dr. Edgar Groenen, Prof. dr. Michel Orrit and Prof. dr. Silvia Völker)
  "Detection of single non-absorbing proteins using a gold nanorod"

Theme 3 'Theoretical Chemistry'

- Dr. Francesco Buda (UL)
  "Modeling key processes in photosynthesis"
- PhD lecture of Kush Singhal (group of Prof. dr. Peter Bolhuis and Dr. Evert Jan Meijer)
  "A molecular dynamics study of chaperone-protein binding"

Guest lectures

- Prof. dr. P. Gros, Professor of Biomacromolecular Crystallography at Utrecht University and winner of the NWO Spinoza Prize 2010
  "Insights Into the Molecular Mechanisms of the Complement System"
- IRTG and PhD lecture of Steffi Roters (WWU Münster)
  "Al-P heterocycles and their reactivity towards small molecules"
- Dr. Sergio Ioppolo (UL), winner Dick Stufkens Prize for the most outstanding PhD thesis
  "*Surface formation routes of interstellar molecules"*

3.3 Seminars

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

April 18, 2011, Leiden University
"*Molecular spin crossover phenomenon: recent achievements and prospects"*;
Dr. G. Molnár
CNRS; Université de Toulouse
France

May 12, 2011, University of Amsterdam
"Silicon Reagents in Asymmetric Organocatalysis"
prof. Pavel Kocovsky
Department of Chemistry, University of Glasgow,
United Kingdom

June 1, 2011, University of Amsterdam
"Towards 'Molecular Movies'. Structural tracking in liquid solution of transient excited states of metal complexes"
Prof. Niels Harrit
University of Copenhagen
Denmark

July 18, 2011, University of Amsterdam
"Fluorescent and Chemiluminescent Squaraine Rotaxanes for Bioimaging"
Prof. Bradley Smith
University of Notre Dame
U.S.A

June 23, 2011, University of Amsterdam
"Charge Transfer in DNA"
Prof. Tetsuro Majima
Osaka University
Japan

June 24, 201, Leiden University
"Metal-based drug against malaria and Leishmaniasis";
Prof.dr. M. Navarro
Instituto Venezolano de Investigaciones Científicas, Caracas
Venezuela

June 30, 2011, University of Amsterdam
"Tetrazines: New molecules and building blocks for functional electrochemically and optically active materials and devices."
Prof. Pierre Audebert
Ecole Normale Superieure de Cachan
France

July 11, 2011, Leiden University
"Modelling the separation of steric and electronic effects of phosphine ligands in Rhodium complexes of N-Aryl-N- nitrosohydroxylamines"
Dr. J. Venter
University of the Free State, Bloemfontein
South Africa

September 9, 2011, Leiden University
"*Designed peptides and synthetic lipid bilayers as models to understand lipid/protein interactions in membranes*";
Prof.dr. J.A. Killian
University of Utrecht, Utrecht
The Netherlands

September 13, 2011, University of Amsterdam
"Scale up of hierarchical zeolite catalysts - Science fiction or science reality?"
Javier Perez-Ramirez
ETH Zurich

September 13, 2011, University of Amsterdam
"Understanding Asymmetric Phase Transfer Catalysis through Chemoinformatics"
Prof. Scott E. Denmark
University of Illinois, Urbana
U.S.A.

September 20, 2011, University of Amsterdam
"Pd-catalyzed polymerizations: large effects induced by a subtle unbalance of the chelating ancillary ligands"
Dr. Barbara Milani
Dipartimento di Scienze Chimiche e Farmaceutiche Universita' di Trieste
Italy

September 22, 2011, University of Amsterdam
"Electron rich molecular clips for hosting neutral electrodeficient guests"
Prof. Piétrick Hudhomme,
Université d'Angers, Laboratoire MOLTECH-Anjou
France

October 4, 2011, University of Amsterdam
"N-Heterocyclic carbenes in catalysis and more: interesting concepts!"
Prof. Frank Glorius
Westfälische Wilhelms-Universität Münster, Organisch Chemisches Institut
Germany

November 3, 2011, Leiden University
"*Discrete metal-mediated multi-chromophore assemblies*";
Dr. E. Iengo
Università degli Studi di Trieste
Italy

October 28, 2011, Leiden University

LIC-Reedijk symposium:

- "*How photosynthesis inspires clean fuels*"
  Prof.dr. H.J.M. de Groot
  Leiden University
  The Netherlands
- *"The coiled-coil connection"*
  Dr. A. Kros
  Leiden University
  The Netherlands
- *"Frontiers in theory of surface reaction dynamics"*
  Prof.dr. G.J. Kroes
  Leiden University
  The Netherlands
- *"Unraveling the mechanisms of genome organization in bacteria and archaea*
  Dr. R. Dame
  Leiden University
  The Netherlands
- *"Protein nanocrystallography by electron diffraction"*
  Prof.dr. J.P. Abrahams
  Leiden University
  The Netherlands
- *"Molecular photovoltaics and mesoscopic solar cells"*
  prof.dr. M. Grätzel
  Ecole Polytechnique Fédérale, Lausanne
  Switzerland

November 11, 2011, Leiden University

MCBIM-minisymposium "*Metals, light, and medicine*":

- *"Photodynamic therapy with multitargeted liposomal zinc phthalocyanine for the improvement of treatment efficacy of solid cancers"*
  Dr. M. Heger
  Academic Medical Center Amsterdam
  The Netherlands
- "*Hybrid imaging agents for interventional molecular imaging*"
  Dr. F.W.B. van Leeuwen
  Leiden University Medical Center
  The Netherlands

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

Colonna, F.
'On the stability of old and novel carbon phases: a computer simulation study'
Prof.dr. A. Fasolino (promotor), prof.dr. E.J. Meijer (co-promotor)
June 8, 2011
Scientist at Fraunhofer Institute for Mechanics of Materials IWM

Duivenvoorden, B.A.
'Synthesis & Biological Applications of Glycosylated Iminosugars'
Prof.dr. H.S. Overkleeft (promotor), Prof.dr. J.M.F.G. Aerts (promotor)
December 15, 2011

Dzik, W.I.
'Group 9 open-shell organometallics: reactivity at the ligand'
Prof.dr. J.N.H. Reek (promotor), dr. B. de Bruin (co-promotor)
January 11, 2011
Postdoctoral Researcher at TU Kaiserslautern

Ernsting, J.E.
'DNA as a scaffold for phosphine-based metal catalysts'
P.C.J. Kamer (promotor), J.N.H. Reek (promotor), P.W.N.M. van Leeuwen (co-promotor)
April 17, 2011
Highschool Teacher Chemistry at Zaanlands Lyceum

Hauwert, P.
'Zerovalent palladium (N-heterocyclic carbene) complexes for transfer hydrogenation of alkynes'
Prof.dr. C.J. Elsevier (promotor)
February 17, 2011
R&D Engineer at Frames

Joya, K.S.
'Molecular Catalytic System for Efficient Water Splitting'
Prof.dr. H.J.M. de Groot (promotor)
December 21, 2011

Knijnenburg, A.D.
'Synthetic modifications of the antibiotic peptide gramicidin S'
Prof.dr. H.S. Overkleeft (promotor)
September 29, 2011
Associate Scientist at DSM Research

Lammers, I.
'Chiral discrimination by phosphorescence'
Prof.dr. C. Gooijer (promotor)
November 14, 2011
Study director Analytical and Physical Chemistry at WIL Research

Linden, W.A. van der
'Towards subunit specific proteasome inhibitors'
Prof.dr. H.S. Overkleeft (promotor)
December 22, 2011

Lutteke, G.
'Studies towards the total synthesis of solanoeclepin A: enantioselective synthesis of the right-hand substructure'
Prof.dr. H. Hiemstra (promotor), dr. J.H. van Maarseveen (co-promotor)
September 29, 2011
Postdoc Leiden University

Mooibroek, T.J.
'The palladium diphosphane catalyzed reduction of nitrobenzene'
Prof.dr. E. Drent (promotor), Prof.dr. E. Bouwman (promotor)
December 22, 2011

Nguyễn, V.A.
'Photoinduces processes in Functionalized and Organized Dye Systems'
Prof.dr. A.M. Brouwer (promotor), dr. R.M. Williams (co-promotor), Prof.dr. Lê Cộng Hòa (co-promotor)
September 21, 2011
Scientist, Hanoi University of Technology

Raja, T.N.
'Fluorescence spectroscopy and imaging of dynamics and microstructure of acrylic polymer emulsions'
Prof.dr. A.M. Brouwer (promotor)
June 14, 2011

Sai Sankar Gupta, K.B.
'Spin torch experiments observed in reaction centers of Rhodobacter sphaeroides'
Prof.dr. H.J.M. de Groot (promotor)
December 22, 2011
Interim-Head of NMR Facility at Leiden University

Schor, M.
'From peptide chains to chains of peptides: multiscale modelling of self-assembling fibril-forming polypeptides'
Prof.dr. P.G. Bolhuis (promotor)
September 20, 2011
Post Doctoral Research Associate at National Physical Laboratory, University of Edinburgh

Smolarek, S.
'UV and IR laser spectroscopy of isolated molecular structural dynamics'
Prof.dr. W.J. Buma (promotor), dr. M. Drabbels (co-promotor), dr. A.M. Rijs (co-promotor)
January 26, 2011
Postdoc in field of optics at Radboud University Nijmegen

Tardioli, S.
'Optical Methods For Structure Elucidation Of Protein-Ligand Interactions: Fluorescence and Ultraviolet Resonance Raman Spectroscopy'
Prof.dr. C. Gooijer (promotor)
November 15, 2011
Terna at -Terna S.p.A-

Warsink, S.
'Palladium complexes bearing nitrogen donor functionalized N-heterocyclic carbene ligands: application in transfer semihydrogenation'
Prof.dr. C.J. Elsevier (promotor)
January 19, 2011

Wawrzyniak, P.K.
'Ab initio modeling of primary processes in photosynthesis: Protein induced activation of bacteriochlorophylls for efficient light harvesting and charge separation'
Prof.dr. H.J.M. de Groot (promotor)
January 26, 2011
IT Consultant for Electronic Payments at Collis

Zeist, W.J. van
'Activating Bonds. Theoretical studies of chemical bonds and their catalytic activation by palladium'
Prof.dr. F.M. Bickelhaupt (promotor)
June 15, 2011
Consultant/researcher at Blonk Milieu Advies

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 R. 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. M.H.M. Janssen (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 (Catexel)
- Prof. dr. J.W. Verhoeven (emeritus UvA)
- Prof. dr. J.G. de Vries (DSM/RUG)

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 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. Matthias Bickelhaupt and Prof. dr. L. Visscher at the VU.

4.2 Annex 2 - Financial Account

Income		**Expenses**	
Contribution UvA 2011	60.000	Personnel Costs	60.879
Contribution UL 2011	6.806	Bureau Costs	1.231
Contribution VU 2011	6.806	Annual Report 2010	2.061
Symposium	1.130	Symposium	5.511
IRTG Contribution to Personnel Costs	999	Re-accreditation process (Peer Review May 2012)	9.045
Interest	988	Courses/Lab visit Leiden	967
		Dick Stufkens PhD prize	1.000
		HRSMC website	252
		Social Activity	1.391
	€ 76.728		**€ 82.336**

Income minus Expenses	**-€ 5.608**
Reservation from 2007	**€ 4.019**
Result 2011	**-1.590**

4.3 – Annex 3 Staff and Temporary Personnel 2011

THEME 1

Bouwman	**HGL**	Bouwman	E.
	HGL-Emeritus	Maaskant	W.J.A.
		Reedijk	J.
	Tenure Track	Bonnet	S.B.
	UD	Fu	W.T.
	PhD	Akerboom	S.
		Bahreman	A.
		Raoufmoghaddam	S.
		Wenker	E.C.M.
		Zheng	S.
	OBP	Albada	G.A.
		Brussel	J.J.M.
		Dijk	J.A.P.P.
	SECR	Snellenberg	Y.
Elsevier	**HGL**	Elsevier	C.J.
	HGL-Guest	Oskam	A.
	HGL-Emeritus	Vrieze	K.
	PhD	Drost	R.M.
		Jansen	E.
		Sluijter	S.N.
	OBP	Ernsting	J.M.
		Tromp	D.S.
Hiemstra	**HGL**	Hiemstra	H.
	HGL BZ	Timmerman	P.
	HGL-Emeritus	Koomen	G.-J.
	UHD	Maarseveen	J.H.
	PhD	Breman	A.C.
		Popovic	S.
		Smeenk	L.
	OBP-Guest	Bieraugel	H.
	OBP	Geenevasen	J.A.J.
Lammertsma	**HGL**	Lammertsma	K.
	HGL-Emeritus	Bickelhaupt	F.
	UD	Ehlers	A.W.
		Slootweg	J.Ch.
	PhD	Boon	L.J.P.

		Dijk	T.
		Rong	M.K.
	OBP	Jong	G.B.
	SECR	Smits-Weijers	M.C.H.
Orru	**HGL**	Orru	R.V.A.
	HGL-Emeritus	Groen	M.B.
	UD	Ruijter	E.
	PhD	Born	D.
		Bouwman	S.
		Graaff	C.
		Kruithof	A.
		Lint	M.J.
		Rombouts	J.A.
		Vlaar	T.
	OBP	Janssen	A.C.
Lammertsma/Orru	**PhD**	Janssen	G.V.
Overkleeft/v.d. Marel	**HGL**	Marel	G.A.
		Overkleeft	H.S.
	HGL-BZ	Boeckel	C.A.A.
	HGL-Emeritus	Lugtenburg	J.
	UHD-Guest	Lodder	G.
	UD	Filippov	D.V.
		Overhand	M.
	PhD	Delft	P.
		Hoogendoorn	J.
		Jong	N.R.
		Li	K.-J.
		Li	N.
		Liu	L.
		Rijssel	
		Walvoort	M.T.C.
		Willems	L.
		Willems	M.
		Wong	
	OBP	Elst	H.
		Meeuwenoord	N.J.
		Nieuwendijk	A.M.C.H.
	SECR	Bruin	C.
Reek/De Bruin	**HGL**	Reek	J.N.H.
	UD	De Bruin	B.

	PD	Lyaskovskyy	V.
	PhD	Tang	Z.
Reek/Hartl	**UD**	Hartl	F.
	PhD	Besset	T.R.M.
		Boer	S.Y.
		Bosch	
		Ciancaleoni	G.
		Daubignard	J.J.M.
		Dydio	P.
		DeRossi	
		Franssen	N.M.G.
		Gumrukcu	Y.
		Koelewijn	J.M.
		Olivos Suarez	A.I.
		Perrier	A.D.
		Terrade	F.G.
		Shultz	A.M.
		Walters	A.J.C.
	OBP	Mahabiersing	Ch.

THEME 2

Buma/Brouwer	**HGL**	Buma	W.J.
	HGL-BZ	Brouwer	A.M.
		Oomens	J.
		Bakker	B.H.
	PD	Wang	Y.
	PhD	Carpentier	C.E.
		Grzetic	J.
		Huerta Viga	A.
		Kumpulainen	T.
		Loop	T.
		Meuzelaar	H.
		Panman	M.
		Rosa Domingos	S.M.
		Tan	E.M.M.
		Liu	K.
	PhD-Guest	Cao	F.
		Chen	H.C.
		Mes	E.M.
	OBP	Groeneveld	M.M.
		Hilbers	M.

		Reinders	P.P.
Buma/Brouwer/Amolf	**HGL**	Bakker	H.J.
		Estruch	T.
Buma/Brouwer/Oomens	**HGL-BZ**	Oomens	J.
	PhD	Alvaro Galue	H.
Gooijer/Ariese	**HGL**	Gooijer	C.
	UHD	Ariese	F.
		Zwan	G.
	PhD	Hooijschuur	J.H.
		Petterson	I.
		Vidami Negoescu	C.
	Laser Technician	Wiskerke	A.E.
	OBP	Buijs	J.B.
	SECR	Cassée	G.M.
De Groot/Buda	**HGL**	Groot	H.J.M.
	UD	Alia	A.
		Buda	F.
		Matysik	J.
	UD-Guest	Cespedes	I.F.
	PD	Ganapathy	S.
		Thomas	B.
	PhD	Eisenmayer	T.J.
		Janssen	G.J.
		Kara	F.
		Miloslavina	Y.
		Monti	A.
		Roy	U.
		Sunku	K.
		Thamarath Surendran	S.
		Vallés Pardo	J.L.
	SECR	Velden	E.
Groenen/Orritt/Völker	**HGL**	Groenen	E.J.J.
		Orrit	M.
		Völker	S.L.
	UD	Gast	P.
		Huber	M.
	PhD	Hashemi Shabestari	M.
		Navarro Perez	P.
		Ruijgrok	P.
		Son	M.

		Yorulmaz	M.
		Yuan	H.
		Zijlstra	P.
	SECR	Leeuwen, van	H.
Janssen	**HGL**	Janssen	M.H.M.
	PD	Niraghatam	B.R.
		Sofikitis	D.
	PhD	Irimia	D.
		Rafiee Fanood	M.
	Laser Technician	Wiskerke	A.E.
	OBP	Tuinder	V.C.M.
Koper	**HGL**	Koper	M.T.M.
UD	Juurlink	L.B.F.	
	Research fellow	Yanson	A.
	Guest	Hongjiao	H.
	PD	Calle Vallejo	F.
		Dudin	P.
		Uka	A.
	PhD	Bashlakov	D.
		Den Dunnen	A.
		Diaz Morales	O.A.
		Hahn	C.
		Kleijn	S.
		Kolb	M.J.
		Kortlever	
		Kwon	Y.
		Rossius	
		Schouten	K.J.H.
		Shen	J.
	PhD-Guest	Yang	J.
	SECR	Dijkzeul	J.
Linnartz	**HGL**	Linnartz	H.V.J.
	PhD	Fedoseev	G.
		Isokoski	A.
Linnartz/VU	**HGL-BZ**	Linnartz	H.V.J.
	PhD	Solovyeva	A.

THEME 3

Bickelhaupt/Visscher	**HGL**	Bickelhaupt	F.M.
		Visscher	L.
	HGL-Guest	Baerends	E.J.
	UD	Gori Giorgi	P.
		Gritsenko	O.V.
	PD	Höfener	S.
		Kazaryan	A.
		Kiewisch	K.
	PhD	Meer, van	R.
		Mentel	L.
		Mirtschink	A.
		Tecmer	P.
		Wolters	L.
	SECR	Jaddoe	S.
Bickelhaupt/ Lammertsma	**PhD**	Mulder	J.R.
Bolhuis/Meijer	**HGL**	Bolhuis	P.G.
		Frenkel	D.
		Meijer	E.J.
	PhD	Du	W.
		Kilic	M.
		Zeiler	R.N.W.
	UD	Dubbeldam	D.
		Ensing	B.
		Vreede	J.
	Guest	Baten	J.M.
	PhD	Brandeburgo	W.
		Diaz Leines	G.
		McKendrick	D.D.
		Nowosielski	M.
		Singhal	K.
		Wolf	M.
		Zhu	L.
	PhD Guest	Colonna	F.
Neugebauer	**HGL-Emeritus**	Hemert	M.C.
	UHD	Neugebauer	J.
	PD	Pavanello	M.
		König	C.
		Kovyrshin	A.
		Solovyeva	A.
Gastlid	**PD**	Goumans	T.P.M.

HRSMC	**OBP**	Zwaan-van der Plas	H.
	SECR	Weijer	R.

4.4 Annex 4 – Publications

Publications Theme 1:

Metals in Catalysis, Biomimetrics & Inorganic Materials (Bouwman, Reedijk, Bonnet, Fu, Haasnoot)

Al-Farhan, K.; Ghazzali, M.; Al-Hazimi, H.M.A.; El-Faham, A.; Reedijk, J.; Hydrogen bonding chains and rings structural motifs in new series of N-phthaloyl aminocarboxylic acid derivatives. Solid state microwave synthesis, structural chemistry, computational calculations and antimicrobial activity, *J. Mol. Struct.* **2011,** *994*, 269-275.

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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
Minimum	**18**

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

Group	Equipment
Bickelhaupt/Visscher	Equipment: Compute servers consisting of Clusters of Linux Workstations.
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
	Elemental analysis (C, H, N, S, Cl), ICP analysis
	Diffuse reflectance spectrometer (300 - 2000 nm)
	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
	IR ATR probe Bruker for in situ IR spectroscopic measurements in solution, 500-2500 cm-1
	UV-vis probe Avantis for in situ UV-vis spectroscopic measurements in solution, 300-1100 nm
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
	Fluoresence 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
De Groot/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 144 cores in total
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) Renishaw Invia Raman Microscope with 532 and 785 nm excitation
	FRED laser for deep-UV resonance Raman spectroscopy.
	Cryogenic setups for high resolution luminescence, Shpol'ski, Fluorescence line narrowing spectroscopy, low-temperature absorption.
	Raman microscope with Kr laser.
	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.
	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.
	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&G PAR, Ametek, Eco-Chemie, EKOM). RRDE.
	Vacuum-tight three-electrode tubular EPR spectroelectrochemical cell.
	UV-Vis-NIR-IR-FIR spectro(photo)meters (Bruker Vertex 70v, Nicolet, Varian, Perkin Elmer).
	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).
	Diode-array UV-Vis spectrophotometers (HP and Scinco S3100)
	EPR spectrometer (Varian) at X-band, suited for LT spectro-electrochemistry
	Time resolved Circular-dichroism/Uv-vis spectrometer with stop-flow equipment
	CHemspeed robot

	Amtec robot for parallel reaction and gas-uptake profiling for kinetics.
Hiemstra/Timmerman	LC-MS instrument
	Several analytical HPLC instruments and one preparative HPLC instrument
	Polarimeter
	Usual equipment for synthetic (organic) research, including ozonolysis apparatus and photochemical equipment
	NMR narrow bore spectrometers frequency range (1H) 400 - 500 MHz
	FT IR instrument
	Prelude™ Parallel Fully Automated Peptide synthesizer
	Freeze dryer
Janssen	Various nanosecond and femtosecond laser systems, hexapole state selectors, molecular beam machines, CCD and delay-line based ion imaging detection systems.
Koper	Various UHV setups equipped with TPD, STM, LEED, EELS, IR, MS
	Electrochemical workstations
	Electrochemical cells combined with FTIR, SERS, STM, MS, HPLC
Lammertsma / Orru	32-node Linux cluster
	250, 400 and 500 MHz NMR equipped with cryoprobes
	Advanced LC and LC-MS machines including preparative LC-MS
	Bruker Daltonics MicroQTOF MS
	FT-IR
	Parallel synthesis equipment, microwave synthesizer, ozonolysis, gloveboxes and other standard synthesis equipment
Linnartz	UHV and cryogenic (10K) equipment / FTIR-RAIRS and TPD-QMS detection / Atom sources / Supersonic plasma facilities / Cavity enhanced and spectrometric (QMS / TOF / Ion trap) detection techniques / IR and UV/VIS lasers
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 / v.d. Marel	LTQ OrbiTrap
	LC-MSMS equipment
	PNA synthesizer
	DNA/RNA synthesizer

	Peptide synthesizer
	HPLC equipment
Wever	1 UV/VIS/NIR absorption spectrophotometers (Cary
	2. Medium speed centrifuges for isolation of enzymes
	3 HPLC systems (one with diode array)
	1 FPLC
	1 High- throughput screening robotics
	1 Laminar Flow cabinet
	1 medium speed centrifuge for centrifugation of microtiterplates