QANU Research Review Chemistry

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Contents:

FOREWORD

This report follows the Standard Evaluation Protocol 2009-2015 (SEP) for Research Assessment in the Netherlands that was developed by VSNU, KNAW and NWO. The purpose of this report is to present a reliable picture of the research activities submitted for this review and to give feedback on the research management and quality assurance.

The review Committee was supported by QANU (Quality Assurance Netherlands Universities). QANU aims to ensure compliance with the SEP in all aspects and to produce independent assessment reports with peer review Committees of international experts in the academic fields involved.

QANU wishes to thank the chairperson and members of the review Committee for their participation in this assessment and for the dedication with which they carried out this task.

We also thank the staff of the units under review for their carefully prepared documentation and for their co-operation during the assessment.

Quality Assurance Netherlands Universities

Mr. Chris J. Peels
Director

Dr. Jan G.F. Veldhuis
Chairman of the Board

PREFACE

An evaluation of the quality of the science performed within the Chemistry Departments at the Universities requires much effort, first and foremost from all the members of the Departments that are being evaluated. The self-evaluation documents, which together with the very important personal contacts and discussions during the site-visits form the basis of this report, are the result of many discussions and careful writing within the departments visited. This is an important first step in a process that should lead to a better insight into the performance of a research group.

The present evaluation report is the result of constructive interactions in a strongly collaborative atmosphere between the staff at the universities and the committee members. As Chair I want to thank all of them for the open, harmonious and hospitable way in which this operation could be brought to a good end.

The quality of chemical research at the Universities is generally very good. The average score for quality of the fifty-eight programmes in this review is 4,2. The score of 4 or 5 ('Very good' or 'Excellent') can only be given to programmes that are nationally or internationally leading and contribute significantly to their field. This means that the scores clearly show that Dutch chemical research is not only a very important national player, but also contributes very substantially to the development of several important areas of the field at the international level. Some programmes are even among the international leaders in their field.

The scores as such do not paint the whole picture. Quality assessment is a multi-dimensional excercise and policy decisions should not be taken without carefully considering the whole context, including the mission, the stage of development and the links with teaching. Societal relevance or 'valorisation' should also not be regarded as a simple isolated criterion. University research aims at maintaining, expanding and disseminating knowledge at the cutting edge of science. These functions are strongly interrelated and should always be carefully balanced.

Strong support is essential for Chemistry to maintain its very high level of quality and to perform its role as an important stimulator of innovation, economic growth and welfare. Full and fast implementation of the joint Sector Plan for Chemistry and Physics will be of major importance for the future development of Chemistry in the Netherlands.

As Chair I strongly hope that the efforts of all involved in this review will contribute to the further success of Chemistry in the Netherlands, in the interest of science and society.

Frans De Schryver
Chairman of the Review Committee

1. THE REVIEW COMMITTEE AND REVIEW PROCEDURES

Scope of the assessment
The Committee was asked to perform an assessment of the research in Chemistry at the University of Groningen (RUG), Wageningen University (WU), Radboud University Nijmegen (RU), University of Amsterdam (UvA), Utrecht University (UU), VU University Amsterdam (VU) and Leiden University (LEI). This assessment covers the research in the period 2001 - 2009.

In accordance with the Standard Evaluation Protocol 2009-2015 for Research Assessment in the Netherlands (SEP), the Committee's tasks were to assess the quality of the institutes and the research programmes on the basis of the information provided by the institutes and through interviews with the management and the research leaders, and to advise how this quality might be improved.

Composition of the Committee
The composition of the Committee was as follows:

- Prof. F.C. De Schryver (chair), University of Leuven
- Prof. S. Larsen, University of Copenhagen
- Prof. J. Michl, University of Colorado
- Prof. J.K.M. Sanders, Cambridge University

Additional members per university:

University of Groningen
- Prof. R.J. Cava, Princeton University
- Prof. G. von Heijne, Stockholm University
- Prof. E.L. Cussler, University of Minnesota
- Prof. Ka Ming Ng, Hong Kong University of Science and Technology

Wageningen University
- Prof. C.E.D. Chidsey, Stanford University
- Prof. H. Hirt, University of Vienna

Radboud University Nijmegen
- Prof. M. Levitt, University of Southampton
- Prof. P. H. Seeberger, Max Planck Institute of Colloids and Interfaces, Potsdam-Golm

University of Amsterdam
- Prof. J. Pawliszyn, University of Waterloo
- Prof. K. Kremer, Max-Planck Institut für Polymerforschung, Mainz

Utrecht University
- Prof. B. Bukau, Zentrum für Molekulare Biologie der Universität Heidelberg
- Prof. B.F. Chmelka, University of California

VU University Amsterdam
- Prof. M. Rowland, University of Manchester and University of California
- Prof. M. Hibert, Université de Strasbourg

Leiden University
- Prof. G.J. Davies, University of York
- Prof. D. Crich, Institut de Chimie des Substance Naturelles (ICSN), Gif-sur-Yvette, France.

A short profile of the committee members is given in the Appendix..

Roel Bennink of the Bureau of QANU (Quality Assurance Netherlands Universities) was appointed secretary to the Committee.

Independence
All members of the Committee signed a statement of independence to safeguard that they would assess the quality of the Institutes and research programmes in an unbiased and independent way. Any existing personal or professional relationships between Committee members and programmes under review were reported and discussed in the committee meeting. The Committee concluded that there were no unacceptable relations or dependencies and that there was no specific risk in terms of bias or undue influence.

Data provided to the Committee
The Committee has received detailed documentation consisting of the following parts:
1. Self-evaluation reports of the units under review, including all the information required by the Standard Evaluation Protocol (SEP), with appendices
2. Copies of three key publications per research programme
3. Results of the bibliometric study on Dutch academic chemistry research 1999-2008, Center for Science and Technology Studies (CWTS), May 2010.

Procedures followed by the Committee
The Committee proceeded according to the Standard Evaluation Protocol (SEP). Prior to the Committee meeting, each programme was assigned to two reviewers, who independently formulated a preliminary assessment. The final assessments are based on the documentation provided by the Institutes, the key publications and the interviews with the management and with the leaders of the programmes. The interviews took place in September 2010 (see the schedule in Appendix C) on location at the Institutes.

Through the interviews with representatives of the research community, the Committee developed an impression of the research programmes submitted for this review.

Preceding the interviews, the Committee was briefed by QANU about research assessment according to SEP, and the Committee discussed the preliminary assessments. The Committee also agreed upon procedural matters and aspects of the assessment. After the interviews the Committee discussed the scores and comments. The texts for the committee report were finalised through email exchanges. The final version was presented to the faculties for factual corrections and comments. The final report was presented to the boards of the participating universities and was printed after their formal acceptance of the report.

The Committee used the rating system of the Standard Evaluation Protocol (SEP). The meaning of the scores is described in Appendix B.

Core of four plus seven times two
The composition of the Committee was particularly complex, because the participating universities and the faculties had decided to have a core committee that would visit all the institutes, plus two additional committee members for each university that the Committee would visit. In view of this complexity, the Committee developed a *modus operandi* aimed at the optimal

use of the expertise in the Committee and at reaching consensus about the scores while taking the overall context into account, with a view to the highest possible degree of comparability across programmes.

Starting from the principle that a review like this is an exercise in constructive criticism, the core members and the university specific members (the "additional members"), were asked to write a preliminary assessment of each of the programmes, in such a way that each programme was covered by a core member, an additional member and the chair. These preliminary assessments were collected by the chair and not communicated in advance to the other members.

During the site visit, before the interviews, the two additional members for that specific university were informed by the chair how the visitation would be handled and what the vision of the Committee was. Just before each programme interview the members were informed of the general trend of the preliminary assessments without mentioning the names of the reviewers. Immediately after each programme interview a consensus based score was given to the programme. At the end of each site visit the subset of scores for that university was compared and again agreed upon by consensus. As the composition was different for each university the core members made sure that, as far as possible, scoring was homogenous and based on the same parameters for all. These parameters included not only the quantitative data provided but also the information obtained during the visit in which especially the past and future scientific vision of a group was probed.

Also in view of the rather complex committee structure, the reporting procedure was structured in the following way. For each University the original draft assessment for a given programme was written by one of the additional members who then sent this to a core member for a first round of editing. The edited texts were sent to the chairperson, who carried out a second round of editing at the university level and attempted some homogenization of style and content. This university specific document was then evaluated and refined by the core members and the agreed text was sent to the additional members for final validation. The general remarks were validated by the core members only.

2. GENERAL REMARKS

Organisational diversity; main focus on programme level
This assessment of the research in Chemistry at the University of Groningen (RUG), Wageningen University (WU), Radboud University Nijmegen (RU), University of Amsterdam (UvA), Utrecht University (UU), VU University Amsterdam (VU) and Leiden University (LEI) covers the period 2001 – 2009 and is based on information provided by these universities in their self-evaluation reports and during the site-visits.

The scope of chemical research is much wider than during previous reviews and includes links with e.g. material science or biology. This has led to a multilayered structure where chemistry, quite often, is embedded in an institute or even distributed between several institutes with a broader mission and with a different emphasis for different universities. In some cases an institute had been recently evaluated, sometimes the chemistry is a rather small part, and in most cases the institutes do not have a classical departmental structure anymore. This has led to a differentiation in the comments related to the Institute, which are in most cases focussed on the future of the Institute, and this also means that a comparison at the Institute's level in the present document is not meaningful.

Homogeneity in all aspects of the evaluation was realized at the programme level and comparison should be restricted to that level.

Finally, this review is of course a snap-shot by a given group of people, with the intent to help the field in its development.

State of the Art; overview of the results
The quality of chemical research at the Universities is generally very good. The Committee scored a total of fifty-eight programmes. The average score for quality of these programmes is 4,2 and no university has less than 4 as the average score for the quality of the programmes. Twenty-three programmes were rated excellent for quality. This indicates that Dutch chemical research is not only a very important national player, but also contributes substantially to the development of the field on the international level.

The second important parameter, viability, indicating the strength and potential of the programmes for the future gave on average for 57 programmes a very good score of 4,2 indicating that, providing that adequate funding remains available, the potential of Dutch chemical research is very good. All universities scored in average 4 or more. Twenty-six programmes were rated excellent for viability. Tenure track systems are now in place almost everywhere. Special programmes to promote gender equality in the academic staff have played an important role together with the use of national (VENI, VIDI) and European (ERC) schemes to attract young scientists in establishing new and maintaining vigorous programmes under difficult circumstances.

Productivity overall equals 4,1. Publication policies are generally sound and emphasize the choice of high quality journals. The number of PhD theses produced is steadily recovering from a dip in previous years and greater attention is now given to finishing the thesis within an acceptable time frame.

The relevance of the research activity is very high with an average of 4,6. Important national and international collaborative efforts, sometimes within the framework of national or European initiatives, have steered research towards areas that are perceived as more directly relevant to

society, most of the time without lowering the quality, as seen above. However, the Committee believes that it is important that room should be left for non-targeted fundamental research.

Dutch chemistry is multidisciplinary and has moved far away from the traditional classification in inorganic, organic and physical chemistry and biochemistry. Biology and materials science are now important components. If one considers the different cluster areas it is pleasing to see that areas that were traditionally very strong in the Netherlands, such as catalysis, including biocatalysis, supramolecular chemistry or materials chemistry including inorganic based systems, have maintained a very high level and installed new and vigorous programmes. Also some of the instrumental analytical programmes such as NMR or scattering techniques are very good to excellent and new strong programmes in mass spectrometry related to biochemistry have emerged.

One area that was traditionally a Dutch stronghold, theoretical chemistry, has retained excellence in the Amsterdam centre and a strong and promising activity in Leiden, but is suffering from downsizing or restructuring elsewhere. Similarly, whereas biopolymer related research is thriving, the classical polymer chemistry, which also had a strong contribution in some non-technical universities, is at present in a state of redefinition.

Several points mentioned in earlier evaluations have to be mentioned again. The chemical research landscape has become too complex. Individual programmes are not only locally embedded in more diverse Institutes, but they are also part of inter-university structures such as TOP schools or large Government, public-private or Science Foundation steered programmes. There is of course the positive aspect of more extensive national collaborations but the downside is that it has become more difficult to set out a clear science policy at the University level. The drive to acquire funding from these initiatives also brings the danger of proliferation of programmes at all Universities. Another danger is that an inward orientation might be fostered too strongly, potentially neglecting the quality that exists elsewhere.

In view of this complexity, the recent realization of a new Sector Plan jointly for chemistry and physics and its implementation is of major importance in the future development of chemistry in the Netherlands. All universities, including the technical universities, have now agreed on priority areas for each specific university. Quite often this is done in such a way that the priorities in physics and in chemistry create an added value because of their complementarity. Even more importantly, the choices have been made with a view to forming or strengthening alliances between different universities, either to ensure the critical mass for a number of topics (such as in the case of the Amsterdam universities), or to realise substantial extra potential through complementarity (such as in the case of Leiden and Delft).

These measures should prepare Dutch chemistry even better in the increasingly global competition in research and for top researchers.

3A. INSTITUTE LEVEL - University of Groningen

University: University of Groningen
Faculty: Faculty of Mathematics and Natural Sciences

The chemistry research in the Faculty of Mathematics and Natural Sciences is embedded in four research institutes:

- The **Stratingh Institute for Chemistry** performs research and teaching in molecular and supramolecular chemistry. Core activities in the chemical sciences, such as bio-organic chemistry, organic chemistry, molecular inorganic chemistry and molecular materials chemistry are embedded in the institute. The institute aims to bridge materials sciences and life sciences research. The research programmes focus on synthesis, catalysis, functional materials, bio-organic chemistry/chemical biology and systems chemistry/complex molecular systems.

- The **Institute for Technology and Management (ITM)** aims to operate at the interface of Engineering Sciences and Business Management with a focus on the technical and engineering aspects of integrated product-process design and development. At present, activities in the area of discrete technology and sustainable chemical process and product technology are embedded in the institute. Both technology areas focus on the application of fundamental sciences in the generation of new product and process concepts, their design and their development and implementation in a business environment. More specifically, the discrete technology research focuses on the creation and development of innovative control systems, while process-product engineering focuses on the design and development of sustainable chemical products and processes based on renewable resources.

- The **Zernike Institute** has as its mission the design and scientific study of materials for functionality. It aims to answer fundamental questions in the fields of functional materials that are relevant for societal problems, and wants to facilitate the transfer of knowledge and overall synergy between physics, chemistry, and biology. The institute approaches problems holistically: from the design, synthesis, and characterization of these materials, to the theoretical modelling and controlled exploration of their properties by fabricating devices. Its strategy is to focus on problems that combine complementary top-down and bottom-up approaches, augmenting the strengths and different areas of expertise of individual groups. To maintain focus, it defined a limited number of new key research areas that relate materials to specific functions.

- The **Groningen Biomolecular Sciences and Biotechnology Institute (GBB)** aims to understand molecular processes of the living cell in relation to their environment. The mission of GBB is to fully understand the regulation, structure, and dynamics of proteins in relation to their function and activity in living cells. These insights in the fundamental properties of biosynthesis pathways, proteins and microorganisms also are relevant for industrial and biomedical applications.

The RUG had not requested an assessment of the Institutes.

3B. PROGRAMME LEVEL - University of Groningen

Programme RUG 1: **Electron Microscopy and Molecular Photobiology**
Programme director: Prof. E.J. Boekema (2003–2009)
Subprogramme leader: Prof. R. Croce (2006–2009)
Research staff 2009: 7.7 fte

Assessments:		
	Quality:	4
	Productivity:	4
	Relevance:	4
	Viability:	4

The mission of the group is to understand the molecular details of fundamental life processes. This is largely done by performing structural studies of the large and transient membrane protein complexes involved in photosynthesis, energy transduction and transport across biological membranes.
The research unit has two main programmes, namely: Electron Microscopy and Molecular Photobiology. The two programmes are linked in the common effort of understanding the complex organization and function of photosynthetic antenna proteins.

Quality
The quality appears very good although not at the international forefront in either of the two focus areas as judged by the relatively small number of their papers cited by their peers as being among the most important in their field. Their citation rate is above average. They are well funded from different sources. The members of this group have been awarded a good number of prizes and invited talks at international conferences. The leadership is overall quite dynamic.

Productivity
This group has published reasonably but not extensively during the period of the review, and can be considered as having very good productivity.

Relevance
Photosynthesis is the key biological energy conversion process. Improving its efficiency or utility may be one of the factors in helping to solve the world's energy supply problems in the post-petroleum era. Therefore this work has in principle high societal relevance. Membership of a consortium "Towards Biosolar Cells" indicates a possible route to valorization.

Viability
The Committee believes that it would be beneficial for this group to develop further its vision for the future of their field, and then work towards the implementation of that vision.

Conclusion
Although the connection between photobiology and electron microscopy was not initially obvious to the Committee, it became clear during the interview that the microscopy work plays an important role in the advancement of the photobiology part of this programme. Therefore their coupling in a single programme is reasonable. This is overall a very good quality programme.

Programme RUG 2: **Membrane Enzymology**
Programme director: Prof. B. Poolman
Subprogramme leader: Prof. D.J. Slotboom (2005–2009)
Research staff 2009: 20.5 fte

Assessments:		
	Quality:	5
	Productivity:	5
	Relevance:	5
	Viability:	5

The Membrane Enzymology group aims to elucidate the mechanisms of signal transduction and small-molecule transport across biological membranes and the role these processes play in the functioning of the cell. The research is directed towards the understanding of the molecular mechanisms driving membrane transport and signaling. A clever and innovative combination of methods in molecular biology, biophysics, bioorganic chemistry and genomics are employed in the research. The activities of the group can be divided into two subprogrammes that work in synergy to achieve the overall goals. One on membrane enzymology led by Prof. Poolman, which primarily focuses on the translocation processes and another in structural membrane biology headed by Prof. Slotboom, which has the focus on the structural and functional analysis of membrane proteins

Quality
Under the very effective and dynamic leadership of Prof. Poolman, the group has established itself as an internationally competitive centre for biochemical studies of small-molecule transporters and other kinds of membrane proteins. The new line of research in cell biology is a welcome development that will widen the scope of the science and open up interesting new possibilities for collaborative projects. The research is supported by the availability of state-of-the-art instrumentation. The Committee finds that significant international and national recognition that the leading senior members of the group have received for their research contributions is fully justified.

Productivity
The group has an excellent publication frequency in the leading journals of the research areas, which is stimulated by the expansion of the group with two younger staff members. There seems to be a steady increase in the PhD-students graduating from the group.

Relevance
The programme is of high relevance for the development of basic membrane biochemistry and for the education of young researchers in a stimulating research environment. In addition the group has taken an active and valuable role in the dissemination of their research to the general public, and serves as an advisor to large and small industrial companies.

Viability
Overall the prospects for the group are excellent. The programme is very well funded and is expanding rapidly. The programme leader is comparatively young and has been successful in having a group of equally committed young scientists join the group. The prospects of the new "Synthetic Biology Centre", which will house the Molecular Enzymology group and other groups with closely related research activities, will create a stimulating environment that beneficial for the development of the group.

Conclusion

The performance of the Molecular Enzymology group is excellent by all the evaluation criteria. It has strong, innovative and highly productive research programme with all possibilities to grow and produce high-level science in the field of biomembranes.

Programme RUG 3:	**Molecular Dynamics and NMR**	
Programme director:	Prof. S.J. Marrink	(2006–2009)
	Prof. A.E. Mark	(2001–2005)
Research staff 2009:	12.5 fte	

Assessments:	Quality:	4
	Productivity:	4
	Relevance:	4
	Viability:	3

The Molecular Dynamics (MD) group concentrates on dynamical simulation of biopolymers and lipid aggregates. The aim is to understand and predict macroscopic behaviour of complex biomolecular systems on the basis of the effective interactions between atoms. In addition, experimental investigation of the structure and dynamics of biomolecules is performed using high resolution NMR.

Quality
This research group has done quite well overall during the review period. Their work is well cited and they have had a significant number of papers in the top 2% in their field. The group has had a fair number of invited talks at international venues and the members have been awarded a significant number of prizes attesting to a good scientific reputation. Some of the Molecular Dynamics programmes that were originated in this group are used world-wide, and this represents a significant contribution to the field. The methods development aspects of the work appear to be very good. The leadership of the molecular dynamics effort is lively and strong. It did not appear that the NMR component of the programme involves methods development, and therefore it appears not to be at the forefront of its field.

Productivity
This group has extensive collaborations with local experimentalists and is actively encouraging a further increase of those efforts. Their research productivity, measured in terms of number of scientific contributions through publications, appears to be very good.

Relevance
Although the issues of protein folding and assemblage in biological systems, some of the main research topics studied by this group, are fundamental science, they are important for understanding biological processes in the long term. Therefore this work appears to have substantial societal relevance.

Viability
The continuation of a distinct NMR research programme at Groningen appears to the Committee to be threatened. In contrast to many institutions, where organic chemists and biochemists are the typical collaborators of NMR groups, at Groningen these researchers either perform their work internally or do work for which advanced NMR methods are not relevant. Thus the NMR part of this programme is likely to fade out in coming years unless a very substantial investment is made in instrumentation and personnel, a decision that should be made by the Groningen administration. On the other hand, the molecular dynamics part of this programme is lively, productive and interesting, and the researchers have a good strategy for continuing growth and viability. The Committee would rate the viability of the NMR programme as 2, and that of the MD programme as 4 or 5, yielding the average score of 3 assigned.

Conclusion

The molecular dynamics group is on an excellent upward trajectory, and their plans to increase the complexity of systems that they can model through ever increasing development of computational and modelling methods is excellent. There presently is little overlap with the quantum chemistry group at Groningen, and when that latter group becomes healthier, such a relationship may prove to be beneficial to these researchers. A future expansion or contraction of the NMR effort should be considered by the University administration, as a mere continuation of the status quo does not appear viable.

Programme RUG 4:	**Protein Crystallography**	
Programme director:	Prof. B.W. Dijkstra	
Subprogramme leader:	Dr. A. C. Terwisscha van Scheltinga	(2010–present)
	Dr. J. Broos	(2005–2009)
	Dr. A.W.H. Thunnissen	(2001–2009)
Research staff 2009:	8.6 fte	

Assessments:	Quality:	5
	Productivity:	4
	Relevance:	5
	Viability:	4

The goal of the group's research is to obtain insight in the functioning of biomacromolecules at the atomic level by means of three-dimensional structure determinations using X-ray diffraction methods, often supplemented by other biochemical or biophysical approaches. Recently, a new research line was initiated on the cholesterol breakdown machinery in Rhodococcus and Mycobacterium tuberculosis.
The main research areas are: enzymes and enzyme mechanisms, protein-macromolecular recognition in various biological processes, functioning of membrane proteins, in particular the mannitol uptake system of *Escherichia coli*, and the molecular basis of the biosynthesis of chitin.

Quality
This high quality group has the equipment required to perform their research, and has been able to obtain significant funding for their work. The group leader has been very productive and is quite well cited. Overall, the citation rate for this group is in the average range for their field, with a relatively small number of publications in the past ten years that can be considered at the top of the field. The group is very well recognized internationally for their contributions to protein crystallography.

Productivity
The publication rate is similar to the average in the field. The group publishes in high quality journals. Their productivity can be considered very good.

Relevance
Protein structure and function are very important areas of research in forefront biological science. The proteins studied by this group are of significant interest. Therefore the Committee judges the work to be highly relevant.

Viability
This group is likely to remain viable in the coming years. They have a good number of young scientists and report that they have all the instrumentation they need to perform their research. They have recently incorporated a new group member whose publication record in recent years is excellent, and this is an important factor in assuring future viability. The current leadership of the group is expected to retire in a few years, providing a good opportunity for a young researcher to take a leadership role. Due to the uncertainty regarding the impending change in leadership, the Committee did not assign this group the highest possible viability score.

Conclusion
This is a high quality research group working in an important area. There is good reason to believe that they will continue to be successful in the future.

Programme RUG 5: **Biotransformation and Biocatalysis**
Programme director: Prof. D.B. Janssen
Subprogramme leader: Prof. M.W. Fraaije
Research staff 2009: 16.9 fte

Assessments:		
	Quality:	5
	Productivity:	5
	Relevance:	5
	Viability:	5

The focus of the research conducted by the Biotransformation and Biocatalysis group is on exploration and engineering of novel and improved biocatalysts. The research ranges from discovery of new enzymes using bioinformatics and metagenomics approaches to detailed mechanistic studies and engineering of enzymes with improved properties. This whole process encompassing enzyme discovery, investigations of the enzymatic function, and the engineering of enzymes for industrial processes is mastered. In addition to these applied aspects the group performs fundamental research in enzymology. The focus has been on enzymes to be used in biosynthesis and degradation of environmental pollutants and xenobiotic compounds. The group is well equipped in terms of research infrastructure and is well embedded in the RUG's chemistry department with valuable collaborations in structural biology and synthetic organic chemistry.

Quality
The group is among the international leaders in the field and has repeatedly shown its ability to push projects all the way from enzyme discovery to practically useful biocatalysts. This highly successful research programme has led to the discovery of several new enzymes of huge environmental importance. Their world leading status in the development of enzymes for biodegradation and dehalogenation is unquestionable. The group is well funded. They are now adding expertise in computational chemistry to try to speed up the process by more "intelligent" design of protein-engineering experiments. The leadership is excellent; overall it is an outstanding group.

Productivity
The group has an excellent publication frequency with publications in the leading journals of the field. It also has a good and steady stream of PhD-theses originating from the group.

Relevance
The research conducted by the group has a high societal impact. The aim is to engineer enzymes that may have industrial applications. Most of the enzymes aim at a cleaner and greener production, and there are several examples of the results of the research that have been commercialized. The unique competences of the group are highly relevant in the education of PhD-students.

Viability
Considering the scientific output, the plans for the coming years, the age structure of PIs in the programme and the substantial funding available, the medium term future of the programme looks very bright. The strategic plans are both realistic and visionary, and include plans that will maintain the research infrastructure at a state-of-the-art level.

Conclusion

The Biotransformation and Biocatalysis group has a strong, highly productive and world leading programme in enzyme discovery and engineering that will continue to produce high-level science.

Programme RUG 6:	**Bio-Organic Chemistry**	
Programme director:	Prof. A.J. Minnaard	
Research staff 2009:	4.3 fte	
Assessments:	Quality:	no score
	Productivity:	no score
	Relevance:	no score
	Viability:	no score

Note: Until November 2007, the group was embedded in the research programme Synthetic Organic Chemistry.

The mission of the programme that was initiated in 2007 is to develop new methods in organic chemistry with particular focus on applications in biological chemistry. Three specific focus areas are homogeneous catalysis, natural product synthesis and chemical biology. The chemical biology work is a new undertaking by the Programme Leader, while the other two areas have their roots in work done during the Programme Leader's time in the Synthetic Organic Chemistry programme. Since the programme just started late 2007 the Committee finds that it is premature to provide explicit scores.

Quality
The quality of the programme leader's published work is very high, although it should be noted that most of his publications date from the time when he was a junior scientist in the Synthetic Organic Chemistry programme and are co-authored by Prof. Feringa. The Committee nevertheless feels confident that Prof. Minnaard will continue to produce high-quality work as an independent programme leader. A good indication of the very good research potential of the group is that it already has attracted a number of externally funded foreign students. The imminent move to the new Life Science is very important as it should allow Prof. Minnaard to expand and deepen his engagement in chemical biology; this being the weakest part of his programme at this point.

Productivity
The group leader has a very good publication frequency in internationally leading journals, but as noted above a relatively high number of these originate from Prof. Minnaard's association with the Synthetic Organic Chemistry Group and has Prof. Feringa as a co-author.

Relevance
The programme is of high relevance both basic organic chemistry, for the understanding of host-pathogen interactions, and for industry. The group leader is the co-author of two patents and has good contacts to industry. The research has already contributed importantly to the chemical biology of *Mycobacterium tuberculosis.*

Viability
The research programme is innovative and of high societal relevance. It has been successful in attracting good funding and has a good strategy for its expansion. The Committee sees no problems.

Conclusion
The newly established group in Bio-organic Chemistry has presented a very interesting and ambitious research programme that judged from the performance of its first two years possesses the potential to be extremely successful.

Programme RUG 7: **Combustion Technology**
Programme director: Prof. H.B. Levinsky
Research staff 2009: 1.1 fte

The programme aims to arrive at microscopically correct and theoretically coherent descriptions of combustion phenomena. It studies elementary physical and chemical processes in high-temperature reaction systems (e.g. flames) and tries to translate the knowledge gained into engineering practice. Financing is shared between the gas company Gasunie/KEMA and RUG.

Due to its very special mission and funding situation, it was found inappropriate to evaluate this programme along the same lines as the other programmes in this review. The findings of the Committee were reported separately to the Faculty and the Executive Board of the University.

Programme RUG 8:	**Synthetic Organic Chemistry**	
Programme director:	Prof. B.L. Feringa	
Research staff 2009:	40.8 fte	
Assessments:	Quality:	5
	Productivity:	5
	Relevance:	5
	Viability:	5

The mission of the research programme is to exploit the full potential of synthetic chemistry to create new structures, functions and chemical systems. The goal is to design novel functional (supra-) molecular materials as well as to develop new catalysts and synthetic methodology. Two areas of interest are defined: Molecular Materials with emphasis on the control of dynamics, and Synthesis and Catalysis with a focus on the development of asymmetric catalysis, catalytic oxidation and application of novel catalytic methods in natural product synthesis and biomolecular chemistry.

Quality
This is a large, world-leading group in the area of supramolecular chemistry. Both the science and the internal organization are excellent as evidenced by citations, grants and the large number of independently-funded young researchers. The leadership is world-class, the lead researcher being very highly cited and internationally recognized through an exceptional number of prizes. The group is highly productive and has made innovative contributions to organic, supramolecular and materials chemistry. A significant number of their publications have appeared in the highest quality scientific journals.

Productivity
This group is at the top of its field in productivity. The large number of individuals is reflected in the very large number of top publications.

Relevance
Innovations in organic catalysis are relevant to many fields of importance to society, in particular to the pharmaceutical industry, and there is some effort in commercialisation. Thus this work is highly relevant.

Viability
This group is highly viable. In addition to their strong senior leadership they also have several excellent younger faculty and researchers and a significant number of graduate students and thus are in an excellent position to continue along their current excellent path into the future.

Conclusion
This is a world-class operation with dynamic leadership and an excellent future outlook.

Programme RUG 9: **Chemistry of (Bio)Molecular Materials**
Programme director: Prof. J.C. Hummelen
Research staff 2009: 5.9 fte

Assessments:	Quality:	4
	Productivity:	5
	Relevance:	5
	Viability:	4

The focus of the research group lies on driving technology in sustainable energy production, micro/nano-electronics, and medicine by creating new electronic materials.

The programme has five subprogrammes:

- Organic electronics
- Molecular electronics
- Molecules at interfaces
- Supramolecular chemistry
- Bench-top Molecular-Electronics

Quality
This program on molecular materials and devices is highly interdisciplinary, with a particularly strong collaboration with one of the Groningen physics groups during the review period. The papers on organic photovoltaics published by this group in the past are very highly cited and practically exploited. The quality of this work has been very good, directed at taking a seminal idea and developing it in a continuing fashion. The group is well funded. However, the success and profile of the group have depended on essentially a single fullerene structure which made a big impact. The current science and future directions of the group leader are not entirely clear, and it is too soon to judge Dr. Chiechi.

Productivity
The productivity of this group has been excellent. They have published a significant number of papers, with a very good number of those in high quality journals. The publication rate has reduced recently.

Relevance
Research on solar photovoltaics of all kinds is of high importance for society. The group has done well in bringing this science into practical application and is making a remarkable effort to instruct the community at large.

Viability
This group has had very good viability but the primary collaborator in physics, a critical part of their research program, has left Groningen. Although long distance collaboration is planned, it is not easy to maintain, so there may be some hurdles to overcome in ensuring the future viability of this program. The young researchers appear lively and thoughtful. The research direction of improving molecular purity and microstructure to improve the function of the devices appears to be a good one, but success in this type of incremental science is not assured.

Conclusion

This is a high quality group, with very good international recognition due to a seminal contribution made to their field in past years. With effort directed at maintaining the collaboration with their physics collaborators, continuing success is possible.

Programme RUG 10: **Physical Chemistry of Polymers**
Programme director: Prof. G. ten Brinke
Research staff 2009: 4.9 fte

Assessments:		
	Quality:	4
	Productivity:	4
	Relevance:	5
	Viability:	3

Research is focussed on the self-assembly in complex polymer systems, involving more than one length scale, often combining block copolymers with supramolecular chemistry. Research efforts involve theoretical modelling, experimental studies as well as synthesis. Theoretical modeling is an important driver for the experimental work. Two subprogrammes are distinguished, one involving fundamental research and the other devoted to the development of applications:

- Theoretical and experimental investigations of self-assembly in complex copolymer systems involving different "competing" length scales
- Development of functional materials from self-assembled comb-shaped supramolecules.

Quality
The self-assembly of two-length-scale block copolymers introduced by Prof. Ten Brinke and his Finnish collaborator Prof. Ikkala has yielded new materials with interesting electric and photonic properties, and has recently been used to manufacture metal nanofoams. The research rests on a solid theoretical foundation. The quality of the science is high.

Productivity
The group has a very good publication frequency in leading polymer science journals.

Relevance
The research is highly relevant for polymer science, especially as it integrates advanced theoretical work with wet-lab studies. The new nano-patterned materials developed in the programme have promising properties that may be exploitable in a commercial setting, but no patent applications have yet been filed.

Viability
The programme leader will retire in a few years, and there is no younger PI in the programme with sufficient expertise in polymer physics to replace him. The Faculty needs to formulate a new strategy for its polymer science.

Conclusion
A high-quality programme which is based on critical expertise in polymer physics. The viability of the programme is poor unless measures are taken to bring in new blood.

Programme RUG 11: **Polymer Thin Film and Surface Science**
Programme director: Prof. A.J. Schouten
Subprogramme leaders: Prof. K.U. Loos
Prof. T. Loontjes
Research staff 2009: 9.6 fte

Assessments:		
	Quality:	3
	Productivity:	3
	Relevance:	4
	Viability:	3

The programme has focussed on the design and study of polymer systems at surfaces and in thin films. It also includes the development of enzyme-catalysed polymerisation reactions. Potential applications include e.g. functional polymer films, prevention of biofilm formation and tissue regeneration. Enzyme-catalysis is a relatively new concept in polymer science, and is worth exploring further.

Quality
The research appears rather heterogeneous and lacks a coherent vision. There are interesting results in some projects, but the overall quality is medium. Impact is low as judged by the number of citations, invitations and prizes. Professor Loos' recent VIDI grant is a positive indicator of potential quality.

Productivity
The productivity in terms of publications and PhD theses is medium, with the most senior staff moving towards retirement and the younger staff not yet fully established.

Relevance
The disparate research areas have clear potential industrial relevance and are also interesting from a more fundamental scientific point of view. A spin-out company has been established to exploit the work of a now-retired member of the group.

Viability
The Programme Leader will retire in a few years, as will Prof. Loontjens. Prof. Loos' work on enzyme-catalysed polymerisations is an interesting niche area attracting industrial interest and with very good potential but it can hardly carry the whole programme. The Faculty needs to formulate a strategy for its entire polymer science programme.

Conclusion
As much of the current work will come to an end in a few years time, the programme needs to be re-structured.

Programme RUG 12: **Polymer Chemistry and Bioengineering**
Programme director: Prof. A. Herrmann
Research staff 2009: 5.8 fte

Assessments:		
	Quality:	5
	Productivity:	5
	Relevance:	5
	Viability:	5

This programme within the field of bio-organic materials focuses on the engineering of bio-macromolecules and bio-organic hybrid structures for medical and technological applications. Work is done on DNA-polymer materials, supercharged proteins to be used as defined poly-electrolytes, and ultra-stable molecular emitters for single-molecule spectroscopy in biology. The group masters a wide range of experimental techniques in the research ranging from organic and polymer chemistry to molecular biology techniques.

Quality
The project leader was recruited to RUG in 2007 from the Max-Planck Institute for Polymer Research, where he was heading a smaller group. Prof. Herrmann research contributions have been recognized with two prizes awarded by the German Chemical Society. At RUG he has very rapidly established himself as an exceptionally creative chemist at the interface between organic chemistry and bio-macromolecular chemistry with an internationally leading research programme. Following the appointment at RUG he has been awarded both a VICI grant (2010) as well as an ERC Starting Grant (2009). His DNA-based nanomolecular designs show great creativity and demonstrate a keen eye for possible applications in areas as diverse as drug delivery and nanoelectronics. A top-quality programme.

Productivity
The productivity is excellent and most of the publications of the group are in the leading journals in chemistry and nanoscience.

Relevance
The programme represents cutting-edge nanomolecular science and points the way for the chemistry of the next decades. The bio-materials resulting from the programme have great medical potential enabling the detection of genes involved in diseases and in drug delivery. The potential commercial application has already led to two patents in the short reporting period. The education of the future generation of researchers is well integrated and an important component of the programme.

Viability
The programme leader has during his relatively short period at RUG established a cutting edge research programme with a group that is well over the critical mass. The funding in the medium term is ensured by the two prestigious research grants. There are clear plans to develop the group's competences in cell biology. The group has established a productive interactions and collaborations to other groups in related fields at the Faculty of Natural Sciences and plans to get similar interactions with the Medical Faculty. The programme is on a good trajectory with excellent prospects.

Conclusion
A very strong cutting-edge research programme in bio-nano science with a great future potential.

Programme RUG 13: **Solid-State Chemistry**
Programme director: Prof T.T.M. Palstra
Subprogramme leaders: Prof B. Noheda
Prof. R. de Groot
Research staff 2009: 8.4 fte

Assessments:		
	Quality:	5
	Productivity:	5
	Relevance:	5
	Viability:	5

The aim of the group's research is to utilize displacive, spin-, charge- and orbital degrees of freedom to control the electronic and physical properties of transition metal oxides and molecular compounds, integrating synthesis of materials in bulk and thin film form, structure studies by surface probe and reciprocal space techniques, and electronic property studies. The objective of the research is to contribute to the fundamental understanding of electronic materials that are technologically relevant for future applications. The research areas are Multiferroic transition metal oxides, Ferroelectric Thin Film research, Orbital Ordering materials and Molecular Materials: Carbon- and O2-based compounds.

Quality
The work of the group during the period of this review has been first rate and is very well respected internationally, as can be seen in the excellent citation numbers and the number of papers they have published in the top 2% of the citations in their field. They are strong in many of the specialist areas that are needed to excel in this field. The head of the group has an excellent international reputation, and appears to direct the focus of the group well. The group is well funded.

Productivity
This group works extensively with experimentalists and theoreticians both in the Netherlands and internationally. They are well connected to the international community of researchers in their field and therefore are on top of the scientific questions in their field. They perform research at international facilities. They have published a large number of papers, many in high quality journals, during the evaluation period. They have presented many talks on their work at international conferences.

Relevance
There does not yet appear to be a clear practical application in current technologies for the materials under investigation. Nonetheless, the scientific questions are at the forefront of the field of condensed matter physics and there are many people world-wide working on this topic due to its scientific importance.

Viability
This group appears to have good plans for continued success, including hiring a young staff member in the specialty area of modern diffraction techniques. Further they hope to expand their capabilities in thin film fabrication; such films are likely the way that the materials they work on would be employed in any future technology. The recent hiring of a new staff member in molecular inorganic chemistry in the chemistry institute will be important for the future work of this group. Also helpful for continuing the viability and high quality of this group would be an additional tenure track position. The general field they work in, "correlated electron materials",

will likely remain an important collaborative research area between chemistry and physics for many years to come.

Conclusion
This is a high quality research group with excellent international recognition, high viability, and good plans for future growth and success.

Programme RUG 14: **Theoretical Chemistry**

Programme directors:	Prof. R. Broer (chair)	(2010-present)
	Prof. M. Filatov	(2005-2009)
	Prof. R. Broer	(2003-2005)
	Prof. J.G. Snijders	(2001-2003)
Research staff 2009:	6.2 fte	

Assessments:	Quality:	no score
	Productivity:	no score
	Relevance:	no score
	Viability:	no score

The theoretical chemistry programme focuses on the development of accurate first principles quantum theoretical methods and their application to problems in chemistry, physics and biology. Research is aimed at the interpretation and prediction of spectra, and also to transition metal and rare earth compounds.

Quality
The group appears to have significant funding and a good young researcher population. Their work is cited at the high average range of research in their field, but they have had relatively few top publications in the past decade. The Committee notes that the group has performed some interesting and creative work in theoretical chemistry, in particular in the area of electronic structure calculations. The investigators argue that one of their primary strengths is very strong collaborations with experimental groups and theorists at other institutes. The group has little international recognition.

Productivity
The publication output during the review period was very limited. The number of publications was small; however the publication performance is seen to be in the high average range according to the crown bibliometric indicator, indicating that this group has made a reasonable number of significant contributions to its field during the period under review. The relatively low number of publications during this review period appears to the Committee to be in large part due to the difficulties described below.

Relevance
The field of study in which this group is engaged, elucidation of the electronic structure of materials, is important for the development of materials science efforts in Groningen and is therefore highly relevant. The work is tied to correlated electron systems, whose eventual applications may have long-term impact on society. The theoretical treatment of chemical systems is a substantial help in understanding experimental observations, and thus theoretical chemistry groups are important in any integrated materials science programme.

Viability
The leadership of this group has changed several times in recent years due to a variety of tragic events and internal issues and is about to change again with the retirement of its current leadership in several years. The Committee believes that a definitive plan should to be put in place to improve the productivity and viability of this programme.

Conclusion
The recent history of the programme is so dramatic, with deaths, incapacitating illnesses, and internal personnel issues, that the Committee thinks it best not to score the programme

numerically. We know that the Groningen administration is aware of the situation. We recommend a continuation of this research group, particularly due to its potential connections to the strong work in materials science in the chemistry division at Groningen. We believe that strong leadership and new early career faculty would be very helpful in improving the viability of this effort.

Programme RUG 15: **Product Technology**
Programme director: Prof. A.A. Broekhuis
Research staff 2009: 6.3 fte

Assessments:		
	Quality:	3
	Productivity:	3
	Relevance:	5
	Viability:	3

The Product Technology group was created in 2003 replacing the Physical Process Technology group. The change in research direction towards chemical product design was accompanied by the appointment of Prof. Broekhuis, who came from a position in industry. Since 2006 he has also been the director of the Institute for Technology and Management. The foci of the group reflect the move of the chemical industry in the Netherlands towards production of higher value-added products. The programme is one of the stronger educational efforts supporting the change in direction, and it includes both product design and product management. There is no research on product management. The main research lines in product design are new chemical products based on polyketone scaffolds and biobased production of chemicals.

Quality
The existing research effort is sensible, with the work on polyketones representing the strongest component. The research produces patents and industrial support. The scope of the work is fairly narrow, a consequence of the small number of faculty involved and their heavy teaching duties. The work on supercritical carbon dioxide, including that on sustainability, seems more a heritage of earlier process chemistry than a topic of immediate value. While carbon dioxide studies did, long ago, lead to a possible process for de-waxing lubes, this was never extensively practiced. Carbon dioxide is a poor solvent for many drugs, so commercial efforts at making drug nanocrystals have largely been abandoned.

Productivity
The papers and patents produced by this group in the reporting period are limited in number. This may be a consequence of the heavy teaching load and the restructuring of the group. The number of Ph.D. students is increasing and this should help the staff involved to become more productive.

Relevance
The value of this programme to the chemical enterprise in the Netherlands is potentially as great as any the Committee reviewed. The new chemical business requires different efforts. The activities of the group are well funded and have led to several patents.

Viability
This group has made a start on this direction, but the start is almost exclusively educational. If it is to be buttressed by research the research activities must go beyond what is currently being done. Such an extension relies strongly on the programme director, who is a veteran of extensive product work in industry, and an effective teacher of this material but his research effort and the research resources are limited. Considering that he is likely to retire in a not too distant future, this programme needs the addition of two other tenured staff members to be truly viable. One of these could come from the existing vacancy; a second could possibly include the replacement for Prof. L.P.D.M. Janssen, who is expected to be replaced by an expert on powders. If these two individuals were to focus their research in areas relevant to the new chemical business, the

programme could become not only the leader in the Netherlands, but key to development of the new chemical industry in Europe.

Conclusion
At the moment, the programme is successful educationally but limited in research. The University should decide whether it wants to continue the education as a holding operation or to extend the programme to a broader product design effort. Doing so has enormous potential but is also with high risk.

Programme RUG 16: **Physical Technology**
Programme director: Prof. L.P.B.M. Janssen
Research staff 2009: 1.5 fte

Assessments:	Quality:	3
	Productivity:	3
	Relevance:	3
	Viability:	no score

This traditional rheological effort is aimed at extrusion with reaction. Studies of extrusion seek to understand how flow varies with applied pressure. For a classical Newtonian fluid, the flow varies linearly with pressure difference, because the Reynolds number is laminar. For polymeric flows, the velocity often varies with a higher power of the pressure because these fluids are shear thinning. If the fluid is reacting while it is extruded, the situation is more complicated. More recent research included efforts on recycling of rubber tires and water purification with rice straw and involves collaboration with other universities.

Quality
The work, which was solid but not spectacular, will probably have a limited impact in the future.

Productivity
The productivity of the programme is reasonable, but a few more publications would have been expected.

Relevance
The value of this programme was strong in the past because it supported products of value in the local region. Because this effort is unlikely to have a large future impact, the Committee agrees with the decision not to continue after the retirement of the present programme director.

Viability
This issue is immaterial since the programme director is retiring and the programme is terminating.

Conclusion
The work in this area was sound and the books produced have some value, but a further intellectual development of this area is not a priority. The Committee supports the University's decision to cease work on this topic.

Programme RUG 17: **Chemical Reaction Engineering**
Programme director: Prof. H.J. Heeres
Research staff 2009: 11.4 fte

Assessments:		
	Quality:	3
	Productivity:	3
	Relevance:	4
	Viability:	4

This group focuses primarily on the reaction engineering of biomass conversion. This includes the catalytic conversion of plant oil to biofuel and other chemicals, and starch to biopolymers. In addition, it works on related technologies such as the use of centrifugal contactors for the reaction of crude oil and methanol, and the subsequent separation into biodiesel and an aqueous stream. The junior researcher, with expertise in traditional catalytic chemistry, is making progress in developing mesoporous catalysts for accommodating the relatively large molecules from biomass. As part of the Institute for Technology and Management, the group explores the process-product relations.

Quality
The research has been widely published in key journals, but citations are relatively limited in part due to the nature of the field. The research group has been able to attract a considerable amount of research funding, and a substantial number of PhD students.

Productivity
The number of publications has been steadily increasing since the current programme leader assumed the position in 2003. All of this bodes well for potentially higher productivity in the near future, although the high teaching load of this research group can be perceived as a possible hindrance to their research output.

Relevance
With the eventual depletion of fossil fuels, biofuels may play an increasingly important role in global energy supply, and the development of novel catalysts and processing technologies is expected to generate significant societal impact. The group has little activity in patenting its work, but has several collaborations through EU networks and with some SME's. They also have longstanding collaborations with several Indonesian universities.

Viability
This group focuses on an important research area of chemical reaction engineering. The research facilities are adequate and the recent research grants amply demonstrate its viability. Whether performance chemicals will be manufactured from lignocellulosic biomass in meaningful quantities remains to be seen.

Conclusion
This relatively young group has a good research record. One of its focus areas on the conversion of the oil derived from biomass implies that most technologies to be developed are close to that of classical reaction engineering although the reactants, a complex multicomponent mixture, come from natural products. Its plan of investigating process-product relations may provide the novelty to propel itself into a leadership position.

4A. INSTITUTE LEVEL – Wageningen University

Wageningen University has one single faculty that consists of five departments:

- Agrotechnology and Food Sciences
- Animal Sciences
- Environmental Sciences
- Plant Sciences
- Social Sciences.

These five departments together contribute to the University mission "For Quality of Life".

The chemistry field is of direct relevance to all departments with the exception of Social Sciences. Aspects of chemistry are part of many research programmes and education curricula. The laboratories that undertake most of the chemistry research and teaching, Biochemistry, Physical and Colloid Chemistry, Microbiology and Organic Chemistry are clustered in Agrotechnology and Food Sciences.

Within the laboratories that are active in the chemistry domain the focus is on the application of chemistry to biological problems. The cluster is represented at the departmental level, where common and collaborative projects as well as investments into large-scale (analytical) equipment such as NMR, GC, LC, MS and fluorescence spectroscopy are being discussed. In part these investments are run by jointly operated centres such as the Wageningen NMR Centre and the MicroSpectroscopy Centre. The chairpersons of these laboratories meet monthly and have a rotating representative that is a member of the Management Team of the Department.

Except for a short introduction, the self-assessment report only contained information on the programme level, because no institutional assessment was requested as this had already been carried out recently.

4B. PROGRAMME LEVEL – Wageningen University

Programme WU 1: **Physical Chemistry and Colloid Science (PCC)**
Programme director: Prof. M.A. Cohen Stuart
Research staff 2009: 18.6 fte

Assessments:	Quality:	4
	Productivity:	5
	Relevance:	5
	Viability:	4

Physical Chemistry and Colloid Science (PCC) investigates how macroscopic properties of systems or materials follow from the chemical nature of matter. PCC focuses on the study of soft matter, which is defined as those systems that respond to forces that are comparable to those that drive thermal motion. Special attention is paid to the colloidal domain. Soft matter problems are studied by combining systematic experimental observations with complementary theoretical analysis. New insights that follow from this strategy are used to deepen the understanding of model systems and develop complex (industrial) applications with relevance for societal needs

Quality
This group has very good quality and has made internationally competitive contributions to important problems during the review period. The experimental and theoretical analysis of the role of ionic strength in the phase behaviour of polymers and colloids is a noteworthy example. The academic reputation of the staff has been and remains high. Cohen Stuart is particularly well recognized in the soft material community, for instance by receipt of the Langmuir Lecture award, the Ostwald medal, and membership in the Royal Dutch Academy of Arts and Sciences. Nevertheless, the group as a whole has not provided world-leading direction in connecting soft matter science to the broader scientific community. One specific area in which the group recognizes that it has limited resources is its ability to prepare new materials and systems. This is one possible direction for future strengthening.

Productivity
The productivity has been excellent. The group has an outstanding strategy for student and staff recruitment, development and productive publication.

Relevance
The overall programme is very relevant to societal needs for soft materials (such as paints and water purification strategies) as well as to the biological focus of WU. It would benefit from a more clearly articulated focus on frontier problems and on the impact of their solution on society.

Viability
The group has a robust and stable research culture in an area of broad relevance to WU in general and to the other chemistry groups in particular. The group will certainly continue to produce very good work. However, there is not yet a plan for the replacement of Cohen Stuart when he retires. The group has suggested an interest in bringing in a new senior member for this purpose, but did not articulate a clear set of goals for how this would be accomplished or what direction this hire would take the programme. Planning for the replacement of Cohen Stuart can provide opportunities for expanded leadership in the field and synergy with other programmes at WU. More focused ties with the neighbouring chemistry and biochemistry groups may provide access to new materials and systems with high relevance to WU and high international impact.

Conclusion

This group is doing very well in an important and clearly relevant area of chemistry, colloid science. The output of high quality publications is steady and the group is well managed. A possible way to strengthen the programme would be the introduction of preparative capabilities to allow work on new materials and systems.

Programme WU 2:	**Organic Chemistry**	
Programme director:	Prof. H. Zuilhof	(April 2008-present)
	Dr. M.C.R. Franssen a.i.	(2007-March 2008)
	Prof. E.J.R. Sudhölter	(2001-2006)
Research staff 2009:	18.5 fte	

Assessments:	Quality:	3
	Productivity:	4
	Relevance:	5
	Viability:	5

The Organic Chemistry programme researches (bio-)organic reactivity, specifically surface-oriented organic chemistry, at the crossroads of nanotechnology, bioorganic chemistry and analysis. The aim is to develop controlled surface modification and use the toolbox of bio-organic chemistry, including biocatalysis, to further develop the area of bio-based synthesis starting preferably from unused agrochemical waste streams as building blocks for bulk synthesis. Novel isolation processes based on miniature devices with controlled surfaces were employed for upgrading waste streams to valuable products

The group has evolved during the review period from containing two quite separate areas (bio-organic chemistry and physical organic chemistry) to a single Chair with a clear focus on surface-oriented organic chemistry relevant to sensing, diagnostics and catalysis.

Quality
The relatively newly-established group on Organic Surface Modification is becoming nationally and internationally recognized and well embedded in graduate schools and Dutch framework programmes MicroNed and NanoNed. This group is also very active as seen by the many collaborations and interactions with other academic groups and industry in the Netherlands. PhD students interact effectively in collaborative projects with biological groups across the campus. On the other hand, the older bio-based chemistry activity is much less ambitious and requires development. Overall, the quality of this group has a clear upwards trajectory, and the score reflects integration over the entire review period.

Productivity
The productivity of the Organic Chemistry programme has seen ups and downs over the past 10 years, with the past few years definitely showing a major improvement with respect to publications and patents. In recent years, Organic Chemistry has been very successful in obtaining major funding.

Relevance
There is clear societal relevance in the surface chemistry programme, with major possibilities for commercial activity. The group has many recent patent applications with a potential spin-off company under consideration. The Group Leader is member of the Boards of NanoNed, MicroNed and MinacNed.

Viability
The Organic Chemistry has only a small number of tenured staff, but has been increasing steadily its non-tenured staff and equipment. By using its human and physical resources wisely, the Organic Chemistry has the tools in hand to further enhance its productivity and quality, particularly in collaboration with biological groups on campus and with industries as diverse as water purification, dairy foods, medical diagnostics and nanotechnology.

Conclusion
This is a young and vigorous group with the potential to expand and flourish within the unique Wageningen environment.

Programme WU 3:	**Biochemistry**	
Programme director:	Prof. S.C. de Vries	(2003-2009)
	Dr. W.J.H. van Berkel	(2001-2003)
Research staff 2009:	14.9 fte	

Assessments:	Quality:	4
	Productivity:	4
	Relevance:	4
	Viability:	5

The research programme in cellular biochemistry aims at understanding the functional role of proteins within living cells. There is a specific emphasis on plant growth regulators and how they activate specific signalling cascades that control plant development. The programme also contains a strong effort enzymology of redox proteins in particular of flavoenzymes. The biological research is supported by the subprogram in analytical biochemistry, which comprises a range of spectroscopic techniques. The multidisciplinary research of this fairly large group is well embedded in the Wageningen University.

Quality
The research programme is internationally competitive, and the investigations of the roles of auxin and the brassinosteroids in plant development are good illustrations of the strong position in plant biochemistry. The work in folding and reactivity of proteins and in the development of metabolite profiling methods represent valuable contributions at the national level, but their impact and strategic importance in the programme in cellular biochemistry are less well articulated. The programme would benefit from greater strategic focus on high impact areas.

Productivity
In the reporting period the group had a very good productivity with frequently cited publications in leading plant and biochemical journals.

Relevance
The research activities are of high relevance to society, exemplified by the investigations of the plant signalling hormones and their link to commonly used pesticides, another example is the development of experimental techniques used in the food and fermentation industry. The very broad range of expertises represented in the research programme is valuable for the education of at all levels at Wageningen University.

Viability
Plant biochemistry is a central and essential component of the mission of Wageningen University. The group is well positioned, particularly with its focus on plant development at the cellular level, and it is well funded. The planned move of the group close to the Plant Sciences building will further strengthen the viability of the group.

Conclusion
The group has made significant contributions to biochemistry and has a promising future in plant development at the cellular level. A strategic focus on high impact opportunities for applying the group's capabilities in protein and analytical biochemistry may enhance the quality and relevance of the programme in the future.

Programme WU 4: **Microbiology**
Programme director: Prof. W.M. de Vos
Research staff 2009: 33.6 fte

Assessments:		
	Quality:	5
	Productivity:	5
	Relevance:	5
	Viability:	5

The programme performs biomolecular research that aims at the discovery of fundamental details on selected microbial model systems, the understanding of the molecular basis of key processes, and the application of the obtained knowledge to develop and optimize processes related to the areas of Food & Health, Bioproducts & Energy, and Environment. The scientific objectives are to unravel the molecular details of the interactions, biotransformations and control mechanisms of selected microorganisms (both bacteria and archaea) and their macromolecules. The research, which is conducted in three groups with complementary expertises focuses on the functional and structural analysis of proteins and nucleic acids at three levels: (i) in situ, (ii) in vivo, and (iii) in vitro.

Quality
The three groups in the Microbiology programme carry out complementary research at the highest international level. The heads of the groups are internationally recognized as the leaders in their fields as can be seen by the list of high prestige distinctions and prizes. Several international collaborations and grants illustrate the strong international position. The Microbiology programme is well embedded in graduate schools and shows high attractiveness to students.

Productivity
Both the publication and the PhD training record show the outstanding productivity of the Microbiology programme at all three levels. Many publications are in high impact journals, and the group has contributed with a number of key reviews in the field. The Microbiology programme has been very successful in obtaining both contract and basic funding.

Relevance
The Microbiology programme is of high relevance to both society and industry, and there is a clear strategy for the technology transfer to industry. It has a strong position in the training of young researchers at WU, and in the development of new research avenues with a great application potential.

Viability
The Microbiology programme has a strong leadership and a transparent management structure. It possesses an adequate number of tenured as well as non-tenured staff. It has a clear strategy for the creation of personal professorships in areas that can complement those already available in the group. The funding ensured by scientific success creates a healthy financial situation that makes it possible to maintain a large number of PhD students in the group. The plans for developing the expertise of the group should ensure that Microbiology programme will maintain the internationally leading position in research and teaching.

Conclusion
The Microbiology group conducts a multidisciplinary and scientifically leading research programme. The track record of the programme is excellent in all aspects. The research

programme in biochemistry based research at the ecological, cellular and molecular level is of high societal relevance and provides a unique educational environment. The research programme is well supported, and the visionary strategy for future developments should ensure a successful continuation of the activities.

5A. INSTITUTE LEVEL – Radboud University Nijmegen

University: Radboud University Nijmegen
Faculty: Faculty of Science
Institute: Institute for Molecules and Materials

1. The Institute

The Faculty of Science of the Radboud University Nijmegen has five research groups. All chemistry groups are part of the Institute for Molecules and Materials (IMM) which was established in 2005 and is currently headed by Prof. E. Vlieg. The IMM conducts research and trains graduate students in the field of functional molecular structures and materials. Emphasis is placed on understanding and controlling complexity in order to design new functionality in these systems.

The aim of the IMM is to design, synthesize, grow, and study molecules and materials in order to understand and control their properties and to design new functionalities. This interdisciplinary field, at the interface of chemistry and physics, is advanced by 21 groups organized along three main themes: 1) Design, synthesis, and growth, 2) Spectroscopy and characterization, and 3) Theory and simulation.

The Committee limits its comments strictly to the chemistry part of the Institute.

2. Quality and academic reputation

Chemistry programme leaders and staff have made successful applications for European Union grants and received international prizes, such as the Humboldt Research Award (Professor van der Avoird, 2008) and the KNAW Academy Chair (Professor Nolte, 2003). In addition, a number of NWO/ECHO and VENI grants have been obtained during the past years. Currently, there are six extraordinary professors affiliated with the chemistry groups of the IMM.

The chemistry groups of the IMM have published about 800 refereed articles between 2001 and 2009. The top 10% of the papers appeared in publications such as Nature PG, Science, PNAS, Journal of the American Chemical Society, Angewandte Chemie, and Physical Review Letters.

The Committee notes that the focus of the chemistry research is on organic and bio-organic chemistry, with very strong national and international positions in supramolecular chemistry, methodology development of NMR and solid state chemistry. The organic section of the Institute strongly interacts with the physics part and has made seminal contributions in the above areas. It has a very high percentage of publications in top journals. It is very well embedded nationally and internationally. It strongly emphasises the potential of applying original findings, which has resulted in a substantial number of spin-offs.

3. Resources

Approximately 70% of the research funds are obtained from external research grants (e.g. Dutch Science Foundation, NWO, EU), contract research and so-called Public Private Partnerships (PPPs). Chemistry staff have also obtained a number of personal grants for fundamental research, e.g. NWO/CW TOP grants for Professors Kentgens (2005), Rutjes (2006), and Van

Hest (2008), VICI grants for Professors Vuister (2005) and Rowan (2006), and VIDI grants for Profs. Rowan (2002) and Cornelissen (2005), Blank (2009), and Elemans (2009)

The IMM houses a number of national and international research facilities, such as a High Field Magnet Laboratory (HFML) for continuous fields up to 33 Tesla (45 Tesla in 2012), European Large-Scale Facility for high resolution liquid NMR, Solid-state NMR Facility for advanced material science among others.
The institute's research infrastructure also includes Laser Laboratories for high-resolution spectroscopy at ultra-short timescales, Velocity map imaging laboratory for studying uni- and bimolecular dynamical processes, and Thin Film Growth Laboratory, where materials and thin films can be grown with atomic precision. Also available are facilities for carrying out advanced synthesis and analyses: instruments for synthesis under extremely high pressure, equipment for combinatorial synthesis, a peptide synthesis laboratory, mass spectrometers, high-performance liquid chromatography facilities, and X-ray diffractometers.

The Committee notes that the section has an excellent record for funding from different national and international agencies. The succession of the Institute's chair and the succession of Prof. Nolte have been very well managed. The Institute continues to attract a high number of PhD's and bachelor and master students. The research facilities are excellent.

4. Productivity

The Committee notes that the production strategy is clear and well-defined and has resulted in a high number of outstanding publications and in the valorisation of the obtained results.

5. Societal Relevance

The IMM is actively involved in bridging the innovation gap, as demonstrated by the number of spin-off companies, such as Chiralix, Encapson, FutureChemistry, Mercachem, ModiQuest, Nanolab, ReRa, SensorSense, Spinnovation, Syntarga, Synthon, and tf2 devices, that have successfully been started in the past decade. Some companies work closely together with a research group, others have grown into independent multinationals. Together they have generated approximately 800 jobs in the region. Many researchers also contribute to general scientific interest magazines, public discussions, and outreach programmes aimed at primary schools.

The Committee notes that the obtained research results are translated into a substantial number of spin-offs. Attention is also given to informing a wider public about the importance of research. This outreach will be further emphasised using the sector plan allocations.

6. Strategy for the future

Chemistry research within the IMM will focus even stronger on life sciences and materials science in the near future. There is also a growing relationship between IMM and NCMLS at the interface between chemistry and biology. The acceptance of the National Sector Plan for Physics and Chemistry causes increased attention to chemical biology. Collaborations on this subject with Leiden University, the University of Groningen, and Eindhoven University of Technology will be intensified in the coming years. Wilhelm Huck (Cambridge University) has recently been appointed as professor of Physical Organic Chemistry.

The focus of the IMM chemistry part of the national Sector Plan Physics and Chemistry is on Chemical Biology. The recent approval of the Sector Plan provides the institute with one full professor and five assistant/associate professors on a permanent basis for this topic. A new tenure-track position is added to the Theoretical Chemistry group.

The Committee notes that the strategic planning for the future looks very good. Further comments are made in the assessment of the individual programmes.

7. PhD Training

IMM's PhD education has a customized modular character. Students and their supervisors pre-agree on which courses the student participate in. The courses are either organised by IMM itself or in cooperation with other (inter)national universities. At the end of 2009, the IMM applied to the Royal Netherlands Academy of Arts and Sciences for the Research School Accreditation (2010-2016). Also, a proposal for piloting a Graduate School for Molecules and Materials (GSMM) was submitted (February 2010) to NWO.

IMM's board provides a Rapid Graduation Bonus for PhD-students who submit their manuscript within the period of employment (4 years for full-time PhD students). To date, 13 of these graduation bonuses have been granted. In addition the IMM and the Faculty are implementing several improvements in monitoring the guidance and progress of the students, e.g. presence of an independent person at go/no-go evaluations and project plan presentations by students at the start of a PhD track.

The Committee notes that the interdisciplinary character of the Institute allows for a broad environment which is optimal for learning and research. The success rate is quite high but improvement may still be possible in the duration of the project until the final graduation of the PhD-student. Discussion with the postdocs indicated excellent interaction between programme directors and their co-workers.

5B. PROGRAMME LEVEL – Radboud University Nijmegen

Programme RU 1: **Analytical Chemistry**
Programme director: Prof. L.M.C. Buydens
Research staff 2009: 4.0 fte

Assessments:		
	Quality:	4
	Productivity:	3
	Relevance:	5
	Viability:	5

The aim of the group is to develop, optimize and validate chemometrical methodologies and strategies for all aspects of data exploration, modeling and interpretation of multi- and mega-variate chemical, biological and medical data and images. The department strives to perform methodological research that is valuable across different application areas together with application-oriented research in which these methods are applied and validated for pioneering science in chemistry and biology. The research programme is designed around 3 areas: Methodological Chemometrics, Spectroscopic Analysis and Spectroscopic Image Analysis, and Molecular Chemometrics.

Quality

This small group carries out very high quality research in a highly specialized area. While it appears to be one of the best groups worldwide in chemometric research, the limited size of the field also limits the number of citations or lecture invitations.

Productivity

Productivity was good early in the evaluation period but there was a substantial decline in publications over several years which is probably due to the small group size. There has been a marked improvement from a very low base in the past two years. Most publications are in specialized journals.

Relevance

This research is of great relevance to a large number of important fields, including metabonomics, imaging, and spectroscopy. The high relevance of this research is recognized by industry through their participation in the major public/private COAST initiative, of which Buydens is a cofounder and board member.

Viability

This research area has appeared to be quite isolated within the IMM and somewhat vulnerable. However the situation has improved significantly. A new tenure-track position has been approved, and the funding stream looks secure in the short term through the promising COAST initiative. Collaborations within the university have improved. The recruitment of suitably qualified PhD students has also taken a significant upturn.

Conclusion

This is a very high-quality research programme in a niche area of great importance to industry and society.

Programme RU 2 : **Biomolecular Chemistry**
Programme director: Prof. G.J.M. Pruijn
Research staff 2009: 8.2 fte

Assessments:		
	Quality:	4
	Productivity:	4
	Relevance:	5
	Viability:	4

The Biomolecular Chemistry group was in the Department of Biochemistry until 2006, when it was incorporated in the IMM. Physically the group is located in building of the Nijmegen Center for Molecular life Sciences (NCMLS) and is also associated with this Center. The research of the Biomolecular Chemistry group is focussed on the post-synthesis processing of human biological macromolecules in particular RNA and proteins, and the alterations in the processes related to stress and in diseases. The group is studying enzymes, enzymatic complexes and other macromolecules that play a role in the post-translational processing. The emphasis is on molecules involved in autoimmunity.

Quality
The research is very good and heavily interdisciplinary. The diversity of the research topics indicate that the group lacks a clear strategic focus and operates opportunistically. Still, the problems tackled are of relevance and the programme is of very good quality. A weakness in the presentation of both the written self-evaluation as well as the presentation was the lack of clear identification of the role of the individuals in the group..

Productivity
The productivity of the group is very good, and a series of high profile papers were produced. In many cases, they are the result of collaborations with a series of other groups, as would be expected from the nature of the work. The reporting period covers 2006-2009, and the self-evaluation report does not contain any information on the number of Ph.D. students in the group.

Relevance
Autoimmune diseases affect the life of millions of people worldwide. The research carried out by the group is that can lead to new diagnostics and treatments is of the high relevance, in particular the work showing that citrullinated peptides are specifically targeted by the autoantibodies of patients suffering from rheumatoid arthritis is of the highest societal impact. The group has a good network and has been active in bringing their results into the therapy.

Viability
The present programme is rather robust and well funded. However as mentioned in the self-evaluation it might benefit from a better overall strategy focusing on long range research goals rather than short term opportunities. The association of the group with NCMLS while being part of IMM can be considered as an opportunity to link the chemical and biological sciences of benefit to the group, though it is accompanied by more administrative work.

Conclusion
The Biomolecular Chemistry group conducts a multidisciplinary and quite diverse research programme primarily targeted towards the diagnosis and treatment of autoimmune diseases. The quality of the research if very good and the group is excellent in bringing their results of high

societal relevance into applications. The programme could benefit from a more strategic focus of the research activities.

Programme RU 3:	**Bio-Organic Chemistry**	
Programme director:	Prof. J.C.M. van Hest	
Research staff 2009:	13.0 fte	
Assessments:	Quality:	5
	Productivity:	5
	Relevance:	5
	Viability:	5

The bio-organic chemistry group aims to create bio-inspired materials and processes to combine the functionality of biological systems with the flexibility and robustness of synthetic structures. Smart hybrid materials are developed based on peptides and proteins, using a variety of synthetic techniques, such as protein engineering, peptide synthesis and controlled polymerization methods. Natural synthetic processes are mimicked by miniaturisation of reaction environments using microsystem technology and by compartmentalization of biocatalysts in polymeric capsules. Research conducted within the Bio-Organic Chemistry group is organized around four themes: Peptide amphiphiles, Hybrid polymers, Nano and microreactors, and Protein-based materials.

Quality
The group produces original and creative research at a high international level at the interfaces of organic chemistry, biochemistry, materials science and nanotechnology. The citation rate has increased dramatically over the past five years and demonstrates the influence of the group's work. Strong collaborations have developed within the IMM together with programmes RU9 (microreactors and synthetic organelles) and RU8 (structure determination of synthetic fibrils by solid-state NMR). Grant funding is strong and well diversified.

Productivity
This is a highly productive group with a strongly increasing number of publications over the assessment period.

Relevance
The programme has high relevance to the development of new materials and processes. The group has also spawned two start-up companies.

Viability
This is a very vital research programme with an accelerating rate of progress. Recruitment of graduate students is good

Conclusion
The Committee considers this a very strong research programme with a bright future.

Programme RU 4:	**Biophysical Chemistry**	
Programme director:	Prof. S.S. Wijmenga	(2002-2009)
	Prof. C.W.H. Hilbers	(2001-2002)
Research staff 2009:	5.3 fte	

Assessments:	Quality:	3
	Productivity:	3
	Relevance:	4
	Viability:	3

Research conducted in the laboratory of Biophysical Chemistry falls within the field of Biological NMR.. Besides Structural and Functional Biology, it includes fields as Metabolomics / Proteomics / Molecular Systems Biology. The aim is to characterize structure and function of biomolecules of medical and biological importance in their natural context. Research is focussed on:

- NMR on RNA/DNA systems of medical and biological importance
- NMR and metabolite and ligand receptor interaction screening
- NMR on Protein systems of medical and biological importance

Quality
This research programme has some international visibility but has suffered since 2008 by the splitting of the group that occurred when Prof. Vuister departed. He had provided many of the key contributions in the reporting period. In the Committee's opinion, the self-image of the residual group is higher than the review would support. The work in the area of nucleic acid NMR is good but not among the best.

Productivity
The productivity of the group is modest and a declining number of coworkers does not help. A collaborative paper in JACS with the solid state NMR group is a good development in efforts to reach out to others and to collaborate.

Relevance
The programme is of societal relevance as the structural work is important for biomedicine.

Viability
The programme has weakened in recent years and appears not to be very viable on its own. It runs the risk of assuming a mere supporting function if no countermeasures are implemented.

Conclusion
This programme was very good but has not recovered from the departure of Prof. Vuister. Its productivity is modest and its future appears uncertain unless it receives attention soon.

Programme RU 5: **Molecular Materials**
Programme director: Prof. A.E. Rowan (2006-2009)
Research staff 2009: 11.2 fte

Assessments:	Quality:	5
	Productivity:	5
	Relevance:	5
	Viability:	5

The aim of the group is the design and synthesis of novel catalysts and materials. The overall group research is systems chemistry (physical bio-/organic chemistry), looking at the relationship between architecture and function. The group focuses on developing the thematic areas of hierarchical materials and novel catalysts from single to cascade systems. Research covers several areas such as:

- Synergetic materials
- Organo- & Bioelectronics
- Single Molecule and Enzyme Kinetics

Quality
The research programme was established only in 2006 but has reached outstanding quality and is in an international leadership position. Prof. Rowan has made strategic hires within his group to cover areas that are important to the evolving programme. The many interactions with other groups are strategically planed as well.

Productivity
The productivity of the group is very high and publications are placed in high ranking journals. As the group is relatively young and still increasing, it is expected that the overall productivity will increase in the coming years.

Relevance
The work is of high societal importance and a spin-off company for one technology has already been established.

Viability
This is a vibrant and healthy programme that will further develop in the future, given the relatively short time of its existence and its rapid rise.

Conclusion
This young programme already is one of the world leaders in "systems chemistry", supramolecular materials and catalysis. It combines synthesis and physical studies in an impressive way. It has numerous international collaborations and a very good publication record.

Programme RU 6:	**Protein Biophysics**	
Programme director:	Prof. G.W. Vuister	(2008-2009)
Research staff 2009:	3.7 fte	

Assessments:	Quality:	no score
	Productivity:	no score
	Relevance:	no score
	Viability:	no score

The Programme director Prof. G.W. Vuister was a member of the Biophysical Chemistry group until 2007, when he became the leader of the Protein Biophysics group. He has established a small research group which contributes to the understanding of protein structure, dynamics and interactions. The aim is to understand biological findings from a structural perspective and to define routes to functional modification and adaptation of proteins and their interacting partners. The research programme is directed towards three very broad themes, fundamental protein properties, regulation of transport and structure validation as part of the NMR technology.
The group employs a wide range of technologies some through collaborations with groups outside RU.

Quality

Despite the diversity the research programme is coherent and addresses important questions in the application of biophysical methods in biology. The research is of high quality with a strong international recognition.

Productivity

The size of the group is close to the critical mass nevertheless is shows a strong publication record with several publications in high- profile journals such as PNAS.

Relevance

A research programme of high relevance to the structural biology and molecular systems biology communities. The provision of tools for NMR structure validation should be highlighted as a particularly important contribution to the worldwide research community.

Viability

Prof. Vuister has accepted a new position in the UK, which excludes that this research group can continue in its present form.

Conclusion

This group has performed very high quality structural biology research, with outstanding contributions to the important area of NMR structure validation. However, the departure of Prof Vuister renders it unlikely that this activity will be continued within the IMM.

Programme RU 7: **Solid State Chemistry**
Programme director: Prof. E. Vlieg
Research staff 2009: 6.4 fte

Assessments:		
	Quality:	4
	Productivity:	4
	Relevance:	5
	Viability:	5

The goal of the Solid State Chemistry group is to obtain a fundamental understanding of the processes that occur during crystal growth (or etching) and to apply this understanding to the prediction and control of crystal properties. Within the field of crystal growth emphasis is placed on morphology prediction, the role of additives and impurities, solid-liquid interfaces, polymorphism, chiral purification, nanowires and protein crystals.

Quality
This is a very good research programme of high quality, and it has introduced some new concepts such as deracemization by crystal grinding. This has aroused world-wide attention. Outside recognition is as yet not very high but the quality of thesis work has been nationally recognized by a number of prizes. It is seen with some concern that the group has shrunk in recent years.

Productivity
The productivity of the group is high, but the Committee believes that the overall output can still be improved considerably.

Relevance
The large number of industrial collaborations provides eloquent testimony to the practical relevance of this group's activities. Polymorphism and chiral purification are important to pharmaceutical companies, morphology of dyes and pigments to other industries. The societal impact of this work is beyond doubt.

Viability
This is a vibrant and healthy programme that will further develop in the future, given the relatively short time of its existence as well as its rapid rise.

Conclusion
This group works in a relatively sparsely populated area of chemistry and does a very good job of it. The broad front approach to the subject is not flashy but is scientifically sound. The Committee was impressed by the vigour of the research group and believes that the approach taken is valuable and viable.

Programme RU 8: **Solid-State NMR**
Programme director: Prof. A.P.M. Kentgens
Research staff 2009: 7.2 fte

Assessments:	Quality:	5
	Productivity:	4
	Relevance:	5
	Viability:	5

The focus of the solid state NMR group is the development and application of nuclear magnetic resonance methods that enable the study of local structure and dynamics in functional materials. The research is structured in three layers. On the highest aggregation level are the applied projects which are mainly focused on macromolecules and materials for energy storage and conversion. Within these projects the structure directing forces and transport and dynamics can be identified as fundamental underlying concepts that we are exploring to gain an in-depth understanding of the principles that bring a specific functionality to a molecular construct or material. This approach requires appropriate methodology and therefore a considerable amount of the research is directed toward enabling technologies with the ambition to progress from bulk characterization to an approach that allows us to unravel the inner workings of the smallest functional units in relation to the processes and functionalities under investigation.

Quality

The quality of the research is internationally leading in several respects. The development of microcoil and stripline techniques for enhancing NMR sensitivity and resolution is potentially groundbreaking. Novel applications have been performed on semiconductor thin films, small single crystals, and on cerebrospinal fluid with a likely impact on metabonomics. There are strong collaborations with other groups at IMM and beyond. Excellent use is being made of the equipment in the Goudsmit Pavilion for NMR and there are promising collaborations with the high-field magnet laboratory with the potential for performing world-unique NMR experiments. The highly specialised and technical nature of this group's developments has led to the work having a lower profile in citations and at conferences than is deserved.

Productivity

The group has a very good publication record with several publications in high-profile journals such as Nature, Phys. Rev. Letters, and J. Am. Chem. Soc. However, although the group has developed much patentable technology, the protection of IP has been weak.

Relevance

The development of new NMR methods with increased sensitivity and resolution is highly relevant to a large number of scientific areas. The group is already involved in numerous collaborations and has demonstrated very promising results in semiconductor research and in metabonomics..

Viability

The group appears to have recovered from past difficulties with the recruitment of qualified PhD and masters students. The funding situation is now promising through the involvement in several high-profile research projects and grants, both on the national and international level. There is excellent infrastructure available and the future looks bright.

Conclusion

This group is very strong intellectually and experimentally, and is now established as a world-leader in microdetector technology for NMR. Applications and collaborations are imaginative and strong. The IMM has contributed to a great deal of this success through excellent engineering support, superb NMR research facilities, and through the provision of an interdisciplinary research atmosphere. The broadening of the research remit beyond classical solid-state NMR should be reflected in a change of title.

Programme RU 9: **Synthetic Organic Chemistry**
Programme director: Prof. F.P.J.T. Rutjes
Research staff 2009: 14.0 fte

Assessments:	Quality:	4
	Productivity:	5
	Relevance:	5
	Viability:	5

The research group aims to develop and apply new catalytic (cascade) reactions to the synthesis of biologically relevant small molecules and to develop and biologically apply novel bio-orthogonal reactions.
One of the research areas involves miniaturization and automation of chemical reactions.

Quality
This is a very good research programme of high quality and potential. The citation rate is rising rapidly but is not yet at the level of international leaders. The approach to project selection currently appears more opportunistic rather than strategic, but the recent appearance of joint publications with biological colleagues is a very promising move in the right direction. The exploration of enzymes in synthesis is also a good future indicator. It is recognized that this programme is still improving and that a more strategic approach will bring benefits in the longer-term.

Productivity
The productivity of the group is excellent: recent years have seen increasing numbers of publications appearing in top journals.

Relevance
The impact of this work on the pharmaceutical chemistry and the chemical industry is evident. Two start-up companies have been created and are developing in a healthy manner.

Viability
This is a vibrant, healthy and expanding programme that appears well-funded and is energetically led. Strengthening collaborations with biological and medical colleagues should provide a strong strategic focus and secure funding stream well into the future.

Programme RU 10:	**Theoretical Chemistry**	
Programme director:	Dr. ir. G.C. Groenenboom	(2008-2009)
	Prof. A. van der Avoird	(2001-2008)
Research staff 2009:	1.3 fte	

Assessments:	Quality:	4
	Productivity:	4
	Relevance:	4
	Viability:	3

The general research theme is the theoretical and computational study of molecular properties, interactions between molecules, and (photo)chemical processes by quantum mechanical methods, as well as the development of new methods, algorithms, and computer programmes. The group is engaged in computational and theoretical study of cold molecules with relevance to studies in molecular traps and to astrochemistry. The research focuses on four related topics:

- Non-covalent interactions:
- Quantum dynamics of molecular clusters and scattering.
- Photochemical reactions in molecules and clusters.
- Cold molecules.

Quality

The group is performing theoretical chemistry research of very high quality. Not surprisingly, the quality dipped after the retirement of Prof. Van der Avoird in 2008. Nevertheless promising new research lines have been developed in cold molecule research.

Productivity

The productivity of the group is very good considering its very small size. Recent collaborative publications have appeared in very high quality journals such as Science and Phys. Rev. Letters.

Relevance

The new research line in cold molecule theory and computations is highly relevant to important research areas such as molecular traps and astrochemistry. The group has the potential of establishing an important position in this niche research area.

Viability

There have been serious doubts about the viability of this research group since the retirement of Prof. Van der Avoird in 2008. At present the group is clearly too small with less than a critical mass for a viable theoretical chemistry activity. However, the recent appointment of a promising young theoretician with an ERC start grant and an independent astrochemical research programme is a very positive development. The research group should now be viable, although vigilance and support from the institute will be required. Long-term viability would be further improved if the group collaborated more actively with the other research groups in the department that have a need for computational and theoretical input, for example RU5.

Conclusion

The group has suffered from instability and lack of personnel since the retirement of the prominent group leader. Nevertheless Dr Groenenboom has established some strong new research directions, and a promising new staff member with an ERC starting grant has been recruited. Still, the group would benefit from a replacement for the vacated chair as the connectivity with many of the other programmes in the chemical part of the institute is weak.

6A. INSTITUTE LEVEL – University of Amsterdam

University: University of Amsterdam
Faculty: Faculty of Science
Institute: Van 't Hoff Institute for Molecular Sciences (HIMS)

1. The institute

The research in the UvA Faculty of Science takes place in ten research institutes. The Van 't Hoff Institute for Molecular Sciences (HIMS) is one of the largest. The mission of HIMS is *"Addressing important issues in science and society through the design, synthesis, analysis, theoretical and fundamental understanding and application of novel functional (supra)-molecular systems with well-defined structural and physical properties and selective reactivity"*.

The HIMS research programme is directed at deepening and broadening our knowledge of matter and of processes on the molecular level. The importance for society is found in applications such as data transport and storage in information technology, efficient transformations of fossil raw materials into useful compounds, analytical techniques for medical, forensic and restorative purposes, and design and synthesis of complex molecules for use as agrochemicals and drugs.

The Faculties of UvA and VU have revised and combined the chemistry programmes of both universities. Key research themes have been defined with a strong focus either at the UvA or at the VU. This will reduce the present five HIMS themes to three.[1] The Sectorplan investment of 2.9 M€ will be used for strengthening themes by adding two new chairs (*Bio-catalysis*, *Supramolecular Separations*) and two new tenured staff positions. An appointment for Heterogeneous Catalysis and Sustainable Chemistry (Rothenberg) was realised in 2008.

The new research themes defined by UvA and VU are:
1. Synthesis & Catalysis (mainly UvA/HIMS expertise)
2. Chemical Biology (mainly UvA/SILS expertise)
3. Analytical Chemistry & Spectroscopy (existing synergy with VU groups)
4. Theoretical Chemistry (ACMM/existing synergy with VU groups)
5. Medicinal, Bio-Organic & Synthetic Chemistry (VU expertise).

In themes 3 and 4 the efforts of UvA and VU are complementary, but differentiation between the universities is obtained by placing these fundamental disciplines in the context of different application areas.

It should be pointed out that the "Art Sciences" group of HIMS was not involved in the evaluation.

Assessment
The Committee supports the stronger collaboration and revision of the chemistry programmes at UVA and VU as this will lead to a better critical mass and in view of already existing synergies to substantial added value. The programmed implementation of this intention within the Sector

[1] The current five themes are: Bio-Molecular Synthesis (BMS, 2 research groups); Catalysis (CAT, 3 research groups); Computational Chemistry (COMP, 2 research groups); Macromolecular and Bio-systems Analysis (MBA, 1 research group in HIMS; collaboration with 2 groups in SILS); Molecular Photonics (MOLP, 1 research group).

Plan will lead to a substantial restructuring of the Institute reducing the present five themes in future to three with strong emphasis on sustainability and energy. The Committee sees a balanced effort, which includes a strengthened computational chemistry programme at UvA, as the only really promising way in the context of the ACMM. The Committee regrets that a promising programme such as Molecular photonics is not profiled more strongly in this restructuring. The Committee strongly supports the Biocatalysis initiative within the Sector Plan as this will strengthen further the already highly successful catalysis group but it cannot judge the impact of the planned chair for Supramolecular Separations as the direction is less clear. Systems Biology was not part of this evaluation.

2. Quality and academic reputation

In the review period HIMS participated in several research schools, technology institutes and networks, such as the National Research School Combination-Catalysis (NRSC-C), the Holland Research School of Molecular Chemistry (HRSMC), the Dutch Institute for Catalysis Research (NIOK), the Dutch Polymer Institute (DPI), NanoImpuls/NanoNed, Catalysis for Sustainable Chemicals from Biomass (CatchBio), Top Institute Comprehensive Analytical Sciences and Technology (TI-COAST). HIMS scientists contribute to policies at the national level through participation in NWO committees and the Royal Academy of Arts and Sciences KNAW. The staff was involved in leading or coordinating many international programmes and projects, especially in the framework of EU programmes. In the coming years the senior staff of HIMS will be increasingly involved in international programmes and projects (such as REVCAT, Erasmus Mundus, the Chinese Academy of Science).

Highlights of external recognition include the prestigious Descartes Prize (2008) awarded by the European Union for transnational collaborative research to the Molecular Photonics group, the testing in 50 cancer clinics in the USA of the cancer drug developed in the group Speckamp (BMS), the Paul Rylander Award in 2006 for the work of Dr. Gadi Rothenberg/CAT on the development of new efficient catalysts for hydrogen oxidation and for the construction of carbon-carbon bond, a Royal Distinction for Prof. Gerrit-Jan Koomen/BMS for his contributions to the field of Bio-Organic Chemistry in 2006, and several Vidi, Vici and ERC grants.

In the period 1999-2008 HIMS published 1602 papers. These publications had an average of 37.5 references per paper and were cited in total 30,767 times. Compared to the journal and field average impact levels, HIMS performs very well.

Assessment
The groups at HIMS perform a very good to excellent quality research in an environment where they are embedded strongly in local and national networks and to some extent in international efforts. There is some interaction between the groups but this could be strengthened. The significance of their contributions and impact is discussed at the programme level.

3. Resources

HIMS had a total research staff of 110,5 fte, including tenured, non-tenured and PhD's. The reorganization of the chemistry department in 2002-2004 resulted in a decrease in staff, followed by an increase in 2007-2009. Direct funding stabilized during the last few years, while research grants and contract research increased. In the period 2001-2009 an average of 6,45 M€ per year was acquired from external funding agencies (on average 16 PhD students + 15 postdocs/year).

In addition, on average 3.5 fte/year tenured staff and technicians were externally funded in this period.

In the summer of 2010 the Institute moved to the Science Park in the Watergraafsmeer. The laboratories for the research groups of Macromolecular and Biosystems Analysis, Computational Chemistry, Molecular Photonics and Biocatalysis are on two floors of the new building. For these groups 1566 m^2 lab space is available. Offices and lecture halls are located in a separate building close to the laboratories. The research groups for Catalysis and Organic Synthesis, including the NMR-facilities, are housed in a separate building with 2052 m^2 available for the laboratories only. This building is connected to the main building in which the other HIMS research groups are located.

Assessment
The move of the Institute to Watergraafsmeer in excellent modern facilities will optimize interaction within the Institute. While number of the tenured staff has decreased over the review period the number of doctoral students has regained the level of 2001 at the end of the review period. The technical and supporting staff has been substantially reduced. This has led to a more balanced budget but still the filling of a number of vacancies had to be postponed in view of resource limitations.

4. Productivity

The number of publications is 180 publications per year for all staff in the themes employed during 2001-2009 and the average output in refereed journal papers per year was close to 13 per fte tenured staff in 2001-2009.

Assessment
The output per fte is very close to the national average but shows a spread between the different groups. Whereas in several groups the choice of top journals is preferred there is room for improvement on this point in other groups. The number of doctoral thesis is more or less evenly spread with positive outliers for the catalysis and computational programmes

5. Societal Relevance

The HIMS groups have many research collaborations with industry and various part-time professors from industry actively participate in the research programmes. HIMS follows an active policy to appoint part-time professors, both internally and externally (from industry). HIMS staff participate in the organization of master classes, educational information meetings and school visits for secondary school pupils to encourage and stimulate their interest in chemistry. Three spin-off companies 'Cat-Fix', 'InCatT', and 'Yellow Diesel' have been initiated in the last years in HIMS and established in the UvA Holding. The institute has various patent applications and also several new projects running that could result in a patent.

Assessment
Attention to intellectual property and its eventual valorization has been initiated in 2006 with a few spin offs already realized. The societal relevance of the programmes will further increase as a result of the restructuring leading to a focus on sustainability and energy.

6. Strategy for the future

Research quality and progress are monitored at the institute level and evaluated by the director. In the coming years this system will be expanded, and regular assessments will take place of the scientific output and awarded funds, contracts, the track record of the research programmes and the researchers. The director will follow a long term strategy of fostering a research culture aimed at original and high impact research in molecular sciences in accordance with the mission of HIMS.

Within the present five themes of HIMS several research groups are of limited size and/or a group leader is approaching the retirement age. To ensure continuity of these groups, the number of themes will be reduced to three and external strategic alliances will be forged.

The renewed focus in the HIMS themes coincides with the priorities that were defined by the Netherlands Organization for Scientific Research (NWO), as published in their Research Strategy for 2007-2010. Subject areas and initiatives of NWO, such as catalysis, micro-reactor technology and complex molecular systems, are fully within the scope of HIMS, as well as the existing programmes in the three areas Medical and Biological Sciences, Physics and Materials Physics, and Sustainability and Technology. The bid of HIMS in the framework of the *Sectorplan Natuurwetenschappen*, together with the VU, is in line with the NWO priorities.

The Faculty has identified Forensic Science as an area where contributions can be made to both fundamental and applied science, e.g. in forensic statistics, information technology, biology and chemistry. The intention of HIMS is to devote part of its research programme to forensic chemistry. In particular the theme of Analytical Chemistry is regarded as well placed to make novel contributions in this field. The Faculty has asked the review committee if this is regarded as a valuable component of the overall research programme of HIMS.

Assessment

The review Committee's comments concerning the strategy related to the Sector Plan are found above The Committee was also asked to comment on the Forensic Science Program, but we received very little information on this in the written submission. We understand that Dr Truyols in the Macromolecular and Biosystems Analysis research group applies his chemometrics expertise within the Forensic Science program, but we do not know how he or his expertise interacts with the biological and other aspects. No clear impression of the direction of forensic research emerged. We are therefore unable to comment in a useful way.

7. PhD Training

PhD students receive extensive training, which is agreed upon at the start of the project. A Research and Education Plan is defined at the start of each PhD project. The Graduate Schools offer advanced training courses for PhD students and post-doctoral research fellows. In addition PhD students are obliged to take a course in teaching. At the UvA, PhD students are obliged to participate in teaching for 25% of their time. PhD students are also stimulated to participate in (inter)-national meetings. To visit an international meeting, a poster presentation, and preferably an oral presentation, is a prerequisite.

Assessment

Comments concerning PhD training will be dealt with in the introductory general remarks at the level of all universities as there is little difference between most universities since most PhD trajectories are embedded in research schools controlling the handling and evolution of students in their schools.

6B. PROGRAMME LEVEL – University of Amsterdam

Programme UvA 1:	**Bio-Molecular Synthesis (BMS)**	
Programme director:	Prof. H. Hiemstra	(2001-2009)
	Prof. R. Wever	(2001-2009)
	Prof. G.J Koomen	(2001-2006)
Research staff 2009:	9.5 fte	

Assessments:	Quality:	4
	Productivity:	4
	Relevance:	4
	Viability:	4

The focus of the Bio-molecular synthesis group is development of efficient and selective, diversity-oriented organic chemistry synthetic methodologies, in particular organocatalytic and biocatalytic procedures, and the target-oriented preparation of molecules of relevance in chemistry, biology and medicine. Research is directed at improvement on these issues through the development of novel catalytic procedures. In the area of target-oriented synthesis the primary goal is the actual preparation of specific molecules for reasons of biological or catalytic properties. The programme is realized by two groups, one in genuine synthetic organic chemistry led by Prof. Hiemstra operating in synthetic methodology and total synthesis, the focus of the other group led by Prof. Wever is on the development of biocatalysts in synthetic organic chemistry.

Quality
The Bio-Molecular Synthesis group has maintained its strong national position throughout the evaluation period despite the increase of the load in teaching and administration experienced by the staff during recent years. The quality of the contributions from the group is very high in their specialized areas. The part time appointment of Prof. Timmerman from Pepscan has strengthened the chemical biology profile of the group. The Synthetic organic chemistry group of Prof. Hiemstra is internationally recognized for its research on synthetic methodology and total synthesis, and the biocatalysis group led by Prof. Wever is internationally recognized for its research in the area of vanadium haloperoxidases.

Productivity
Overall the productivity of the group is very good considering that the limited funding opportunities have reduced the number of Ph.D. students in the group. There is room for an increased productivity in the new developing areas.

Relevance
The decrease in pharmaceutical industry in the Netherlands has a negative impact on the job opportunities for the students graduating from the group. Small size companies are a good alternative for collaboration, commercialization, funding and employment. The group has initiated collaborations with small companies to address the loss of the presence of larger pharmaceutical companies in the Netherlands

Viability
Though the Sector Plan should offer good opportunities for the future, the group is encouraged to get other external funding that could help to replace the aging equipment. It is vital for a successful continuation of the biocatalysis research programme that the plan for the succession

of Prof. Wever is not delayed but realized as soon as possible. Appointment of another part time professor working in industry might further strengthen the viability of the group.

Conclusion
The research carried out in the Bio-Molecular Synthesis group is of a high standard and good productivity with significant industrial relevance. To ensure a productive continuation of the research programme it is important that the plans for replacement of the senior staff are realized.

Programme UvA 2:	**Catalysis**	
Programme director:	Prof. C.J. Elsevier	(2001-2009)
	Prof. J.N.H. Reek	(2006-2009)
	Prof. G. Rothenberg	(2008-2009)
	Prof. P.W.N.M. van Leeuwen	(2001-2007)
Research staff 2009:	35.9 fte	

Assessments:	Quality:	4
	Productivity:	5
	Relevance:	5
	Viability:	5

The catalysis group is large and flourishing. It successfully explores a broad range of homogeneous and heterogeneous catalytic areas in the academic arena and commercializes them via spin-off companies or existing chemical industries. The synergy between the research groups, various industrial partners, that sponsor the research projects, and spin-offs facilitate progress towards achievement of the main objectives, which include the development of new catalytic processes that are sustainable, atom-economic and show high chemo-, regio-, and stereo-selectivity. A strong focus is on the development of novel concepts in catalysis, including supramolecular catalysis, bio-inspired transition-metal catalysis and complex catalysis.

Quality
The Catalysis group maintained a strong international presence throughout the evaluation period. The group consists of three components: the homogeneous catalysis subgroup presently led by Professor Reek and focusing on supramolecular approaches to transition metal catalysis has had an exceptional global impact; Professor Elsevier's sub-group, exploring the synthetic organometallic chemistry of the late transition metals has made substantial contributions using carbyne ligands for catalysis; Professor Rothenberg's heterogeneous catalysis group is interested in sustainable chemistry. These three groups are planning to form a Catalysis Centre of Excellence in the near future.

Productivity
Scientific publications are numerous, frequently appearing in top international journals, and are highly cited. The members of the team are recognized by international awards, they are members of Editorial and Advisory boards of several journals and they actively participate in organizing international symposia and meetings. The contributions made by the younger members of the team are increasing.

Relevance
The development of new catalytic processes with the potential for scale-up in an industrial setting is a key contributor to the future sustainability of modern society. This is recognised by the group, which displays a strong priority to commercialize the outcomes of its research. A small company has already begun operation based on discoveries made in the group.

Viability
There is an excellent potential for this theme. All members of the group are pursuing strong ties with industry. They are actively developing young faculty and are a fruitful source of training for graduate students. Whatever facilities are missing at University of Amsterdam, are available via the Catalysis group at the University of Utrecht.

Conclusion

The catalysis theme has developed a substantial momentum. Its strengths and accomplishments are recognized within the Netherlands and internationally by the scientific community. The staff members of the catalysis theme are involved in various European networks, including IDECAT, the European network of catalysis. The catalysis theme is complementary to the research themes pursued at the VU, and this is expected to result in future expansion of the collaborations between both institutions.

Programme UvA 3:	**Computational Chemistry (COMP)**	
Programme director:	Prof. P.G. Bolhuis	(2007-2009)
	Prof. R. Krishna	(2001-2009)
	Dr. E.J. Meijer	(2007-2009)
	Prof. B. Smit	(2001-2007)
Research staff 2009:	16.0 fte	

Assessments:	Quality:	5
	Productivity:	5
	Relevance:	5
	Viability:	3

This group's research in computational chemistry can be characterized by two terms, namely scale bridging and interdisciplinarity. Quantitative and qualitative understanding of complex biological or synthetic materials requires a linking of chemical aspects (local structure of molecules, quantum chemical properties) to macroscopic/generic behaviour. In computer simulations this requires the use of many quite different numerical approaches dealing with different time and length scales and the ability to link them systematically. Such multiscale modeling is the hallmark of the recent methodological work of the group, as well as the main thrust of anticipated future activities. This is complemented by close interactions with a variety of different experimental groups that provide the interdisciplinary input for applications of the theoretical work. In turn, the applications foster further method development.

Quality
Computational chemistry at UvA has an excellent scientific reputation due to a continuous output of important results, which have been at the forefront of science in the international competition. Having excellent scientists with rather different backgrounds working on rather different topics within the same group created the setting for a very successful programme. It also has offered unique opportunities for interactions to the benefit of projects and students. Due to the departure of Smit and Frenkel, recently the focus has shifted somewhat toward scale bridging approaches and transition path sampling applied to bio-macromolecular studies (Bolhuis). This is complemented by careful atomistic and quantum chemical studies. In summary, the group maintained a very high level of performance while concentrating on new topics.

Productivity
Over the last ten years the productivity has been very high. Many of the papers have been published in top journals. Considering the change in the number of scientists involved, the output has been very high while maintaining the high quality. The number of PhD students in theory generally is somewhat smaller compared to other chemical disciplines, but in the present case it is adequate.

Relevance
The relevance of publications is demonstrated by the quality of journals and the high rate of citations. In addition the UvA group is a highly respected host for external visitors, postdocs and PhD students. The annual simulation school attracts students from all over the world and close interaction with pure and applied experimental physical chemists guarantees that the new results and insights find their way into the "real world". A good balance between method development and applications ensures the recognition of results in the relevant communities.

Viability

The computational chemistry programme gained the reputation of an international top programme under the leadership of (most notably) D. Frenkel, B. Smit and R. Krishna (with D. Frenkel only part time at UvA, main position at FOM). The group has enjoyed excellent viability not only through these group heads but also through very good scientific staff. This robustness against personnel fluctuations and the related broad basis of funding income was weakened by the departure of D. Frenkel, B. Smit and A. L. Fasolino, and is threatened even more by the upcoming retirement of R. Krishna. With the appointment of P. Bolhuis as Professor of Computational Chemistry an important step to sustaining the quality of the programme has been made. He is presently supported by very good staff, partly from the other subgroups. However this might not be sufficient to support new research directions while at the same time keeping the highly desirable scientific breadth.

Conclusion

The computational chemistry group is first rate measured at an international level. It is however in a transition period, having experienced substantial changes and losses during the last few years and expecting the retirement of another professor in 2011. The appointment of P. Bolhuis was an important step to maintaining continuity and the scientific quality and to further developing the computational chemistry at UvA. However, to maintain continuity of excellence in this broad field and to support and strengthen this effort it is extremely important to immediately start the search for a successor of B. Smit with a research focus complimentary to that of the Bolhuis group. This also has to be seen in the context of the Amsterdam Chemical Multiscale Modeling (ACMM) initiative and the coordination of the chemistry programme with the VU. The Committee sees a balanced effort, which includes a strengthened computational chemistry programme at UvA, as the only really promising way.

Programme UvA 4:	**Macromolecular and Biosystems Analysis (MBA)**	
Programme director:	Prof. P. Schoenmakers	(2001-2009)
	Dr. W. Th. Kok	(2001-2009)
	Prof. A.K. Smilde	(2001-2003)
Research staff 2009:	19.1 fte	

Assessments:	Quality:	4
	Productivity:	4
	Relevance:	5
	Viability:	3

The group is built around areas of expertise including separations and data analysis. Part of the research conducted is technology-driven, directed at unravelling the fundamentals of new separation techniques, while part is application-oriented, directed at the development of analytical techniques and methods for the characterization of specific samples. The Analytical chemistry group explores new or greatly improved methods for the separation and characterization of complex mixtures, with special attention on natural and synthetic macromolecules. There is the intention to develop aspects of forensic science.

Quality
The part of the programme focusing on separations is quite successful. The leader of the group, Prof. Schoenmakers, is recognised internationally as an expert in the field of chromatography, particularly in the area of multidimensional chromatography as applied to the separation of polymers, while Prof. Kok is recognized for his contributions to capillary electrophoresis. The junior member of the group, Dr. Vivo Truyols is initiating work in chemometric data processing, but it is too soon to assess its quality or impact. Special Chair, Prof. Janssen, who is a research leader at Unilever, is an accomplished researcher but his academic contribution is unclear.

Productivity
The group has published a number of cutting-edge contributions to multidimensional separations and micro analytical systems, and these are well cited. The absolute number of publications is relatively small considering the group size.

Relevance
The analytical science developed by this group, and the trained young analytical scientists they produce, are all highly relevant to the needs of industry. Indeed the demand for these students is so high that some students leave to take up positions before completing their theses. Truyols' contribution to the new MSc in Forensic Science may also provide relevant training, but we were given no evidence of this.

Viability
UvA has nominated analytical chemistry as one of its priority areas within the sector plan. Considering that a claimed focus of this group is applied mass spectrometry, it is surprising to note that the expert in this area is not employed at the Institute but is embedded in the Swammerdam Instituut voor Life Sciences (SILS). The Committee was not in a position to evaluate the effectiveness of the interactions. The Committee felt the need for a clear long-term plan for the strengthening and necessary diversification of the present programme. There are good opportunities for synergies with the analytical chemistry programme at VU and for participation of the theme in the emerging analytical-science (TI-COAST), nanotechnology programmes and potentially forensic-science (NWO).

Conclusion

There are existing strengths in separation techniques but also major challenges around the apparent lack of long-term planning. Productive collaboration and sharing (or merger) with VU should be pursued vigorously. The Committee did not receive clear evidence of emerging in-house forensic research.

Programme UvA 5:	**Molecular Photonics**	
Programme director:	Prof. A.M. Brouwer	(2001-2009)
	Prof. W.J. Buma	(2001-2009)
	Prof. L. De Cola	(2001-2004)
	Prof. J.W. Verhoeven	(2001)
Research staff 2009:	22.1 fte	

Assessments:	Quality:	4
	Productivity:	5
	Relevance:	4
	Viability:	5

The Molecular Photonics team aims to advance the fundamental knowledge of the dynamics of excited states in molecules and nano-sized objects, and to contribute with its expertise to applications in the photosciences. The research programme in molecular photonics developed in time from a focus restricted to small molecules or fragments of molecules towards the interplay of molecular excitations and molecular conformation/structure. The group's work on complex molecular systems is mostly based on a variety of spectroscopic techniques developed for smaller molecules, while modern near-field optical methods have not been widely used so far. Rotaxanes have served as model systems for further development. Currently, the group closely interacts with other activities in the HIMS such as Bio-molecular Synthesis, Catalysis, Macromolecular Biosystems, and Computational Chemistry. It provides the optical spectroscopy expertise and knowledge necessary to understand the link between properties/effects and molecular structure and function.

Quality
With the early retirement of Prof. J.W. Verhoeven in 2001 and the departure of Prof. L. De Cola from UvA in 2004 the two most visible scientists of the Molecular Photonics Programme were gone. With W. J. Buma and A. M. Brouwer now heading the programme, a stronger concentration of effort toward larger functional molecular systems has led to a more focused programme with many interactions within the HIMS and further national initiatives. Work on light responsive motor molecules is of very high quality and points towards the important general direction of linking spectroscopic properties, such as a vibrational spectrum, to molecular mechanisms that determine functional properties. Along this path the group is on a good way to further improvement of its already high quality in the future.

Productivity
The output of publications is in the typical range for a very good experimental group. A significant increase, without considerable addition of personnel, which regretfully is not envisaged in the Sectorplan, would most probably be at the expense of quality. By far most of the papers are excellent and appear in first rate journals, with quite a few in general top quality journals.

Relevance
The publications of the group are well cited and valued by the scientific community. They address basic physical and physico-chemical properties of molecular systems, which are at the centre of scientific interest, but also of societal needs in that they address molecular mechanisms important for advanced catalysis research (nanostructures, water splitting …), health related aspects, or soft matter materials science.

Viability

After the departure of Verhoeven and De Cola the group regained stability around WJ Burma and AM Brouwer. It is on its way up and has been honoured by the Descartes Prize for Transnational Research in 2008, and the highest quality is now within reach. The group enjoys very fruitful collaborations at the local and international levels. In providing key spectroscopic expertise at the HIMS it plays a central role also locally. With new junior members new research topics can be approached making the group even more indispensable in the local setting. The group has the ability to attract excellent junior members and a high earning capability. Further subfields, not directly represented in the core group, are well represented by external collaborations via "professor by special appointment" (Bakker, Oomes).The Molecular Photonics programme appears to be vital, strong and stable.

Conclusion

After suffering two severe losses the molecular photonics group has demonstrated its viability over the last few years and is well on its way to regain the old excellent reputation. The productivity is excellent and the restructuring of the programme together with the appointment of new junior members as well as the formalized external contacts to AMOLF, FOM Rijnhuizen are excellent indicators. Focusing on the relation between spectroscopic properties and specific molecular function makes the group an ideal and crucial scientific partner for other groups in the HIMS and beyond. Strengthening the rapidly developing new photosciences methods within the Molecular Photonics Programme would complement the methodological portfolio and further improve the standing of the group.

7A. INSTITUTE LEVEL – Utrecht University

University: Utrecht University
Faculty: Faculty of Science
Department: Department of Chemistry
Institutes: Bijvoet Institute of Biomolecular Research
Debye Institute for Nanomaterials Science

1. Structure

The Department of Chemistry is one the six departments in the Faculty of Science. The other departments in the Faculty are Biology, Informatics, Mathematics, Pharmaceutical Sciences, and Physics and Astronomy.

The research profile of the Department has interlinked multidisciplinary research lines and is in line with the research profiles of the Faculty of Science and of the university, including the UMC Utrecht. The Department combines advanced imaging technology (mass spectrometry, NMR, X-ray) with biochemistry. There are numerous collaborations with UIPS, UMC Utrecht, the Faculty of Veterinary Medicine, the KNAW Hubrecht laboratory, and the settlement of Danone Nutrition in 2012, all located on the Utrecht Life Science Campus. Within the Faculty of Science not only natural sciences and life sciences, but also fundamental and applied research co-exist and re-enforce each other.

The Department conducts research in biochemistry, biomolecular structure, colloids, nanophotonics, catalysis, and hard and soft condensed matter. Its research is based on three pillars:

1. Biochemistry and Structural Biology: Research into the structure-function relationship of biomolecules (Bijvoet Institute).
2. Nanomaterials: Research into the physics and chemistry of interfaces and nanomaterials (Debye Institute)
3. Energy and Sustainability: Research into energy and sustainability issues (Copernicus and Debye Institutes).

Only the research programmes of the Bijvoet Institute and the Debye Institute were submitted for this Chemistry review.

The **Bijvoet Institute for Biomolecular Research** aims to further fundamental insight into the relation, at the molecular level, between the structure and the function/activity of biomolecules that are involved in recognition, interaction, and regulatory processes. The Bijvoet Institute is part of the Utrecht Graduate School of Life Sciences.

The **Debye Institute for Nanomaterials Science** has as its scientific mission to facilitate and promote leading fundamental and applied research in nanomaterials science with particular emphasis on colloids, nanophotonics and catalyst materials and its potential for realizing a more sustainable society. The Debye Institute is part of the Utrecht Graduate School of Natural Sciences.

The Department of Chemistry offers a mono-disciplinary Chemistry curriculum for bachelor students. The Bijvoet Institute participates in the 2-year multidisciplinary master program "Molecular and Cellular Life Sciences" of the Graduate School of Life Sciences and the Debye

Institute organizes the 2-year multidisciplinary master program "Nanomaterials: Chemistry and Physics" of the Graduate School of Natural Sciences.

In 2010/2011, several groups of the Department of Chemistry are scheduled to move into a new laboratory building, to further increase cooperation and visibility. The building is adjacent to the laboratories of the UMC Utrecht and the Faculty of Veterinary Medicine. The groups that will go into the new building are: Medicinal Chemistry and Chemical Biology (UU04), Biochemistry of Membranes (UU07), Inorganic Chemistry and catalysis (UU10) Organic Chemistry and Catalysis (UU8) and all groups of Pharmaceutical Sciences. In this manner, for example the Catalysis Centre Utrecht (CCU) will be under one roof, strongly enhancing interactions between the programs UU08 and UU10.

Other measures regarding the research programmes include:
- The programme UU12 (Theoretical Chemistry) will be discontinued and brought into programme UU09 (Condensed Matter and Interfaces).
- Cooperation between the research programmes UU04 (Medicinal Chemistry and Biology), UU07 (Biochemistry of Membranes) and UU08 (Organic Chemistry and Catalysis) is organized in the Chemical Biology Centre Utrecht.

2. Societal Relevance

The Department of Chemistry has a specific policy for the valorization of research. Patents, patent applications and spinout activities are regarded as the main output of the valorization efforts. Numerous examples of this type of output are given in the self-assessment report, not only in the more applied research, but also in the fundamental research. Patent rights can be jointly owned, transferred to an industrial partner or commercialized in spinout activities.

Almost half of the PhD's continue their careers in Industry after graduation.

3. Strategy for the future

As noted in the self-assessment report, the financial situation in the Faculty endangers the continuity of research, because the more experimental facilities and programmes rely almost entirely on competitive funds and contracts (2nd and 3rd stream). The ratio of permanent staff over temporary researchers is very low in many UU-programmes. Since 2005 the number PhD students directly funded from the university has decreased strongly. In recent years several thematic groups in the membrane and oligosaccharide field have been discontinued and biomembranes research merged into chemical biology.

On the positive side, the financial impulse of 10-20 million Euros yearly with the Sectorplan Physics and Chemistry can be noted. The Department also expects that the cooperation with industrial partners will increase. The Science Park Utrecht will mainly house companies in the field of life sciences. Danone-Nutrition will set up an innovation centre for specialised food products in 2012. This decision was influenced by the existing cooperation with Pharmaceutical Sciences and University Medical Center Utrecht.

The Department expects to increase the collaboration with Pharmaceutical Sciences (UIPS), which will be housed in the same new building as many chemistry groups. Energy research is also mentioned as a new area for profiling the chemistry research, especially in the Debye and Copernicus Institutes.

Within the scope of the Strategic Plan for Physics and Chemistry (SNS, *Sectorplan Natuur- en Scheikunde*) the Department of Chemistry wishes to strengthen three focal point research areas: (A) structural biology, (B) catalysis and (C) colloids. The SNS will help to realize these ambitions since it allocates structural money to appoint new research positions at the level of professor as well as assistant/associate professor in these three focus areas.

(A) Research in **Structural biology** will be enforced with a new research group in single-particle electron microscopy (with one full professor, associate professor and technical assistant). It is the objective to appoint another associate professor in this research line on 'electronic microscopy of large dynamic assemblies'. The Department aims to concentrate its activities in structural biology and molecular life-sciences, while seeking opportunities to expand in areas like molecular electron microscopy/ tomography and chemical biology.

(B) **Catalysis research** will be further strengthened by the formal creation of a Catalysis Centre Utrecht as all catalysis groups will be housed in the new Leuvenlaan building. Research focus will be expanded by the appointment of at least one full professor in the area of ***organic-based porous catalysis materials***, a technician and probably one assistant professor. By doing so the organic and inorganic synthesis activities will be interconnected leading to the synthesis, characterization and use of new functional porous materials. It also aims at the extension of its research line in nano-scale spectroscopic imaging of porous materials with an assistant professor and a technician.

(C) It is the ambition of the **Colloids research** group to expand their research lines towards patchy colloids, interactions between quantum dots, and new magnetic systems. By doing that, collaboration with the groups of Profs. Vanmaekelbergh and Meijerink (chemistry) and the Soft Condensed Matter Group of Profs. Van Blaaderen / Dijkstra (physics) will be strengthened. In the SNS, extension of the research staff by an assistant professor has been applied for.

The Department will increase the focus on *Energy for Sustainable Development* through closer collaboration between the researchers of the Copernicus Institute and the Debye Institute (both the chemists and physicists). The activities will also be part of the UU focus and mass program *Earth and Sustainability*, focal point *Sustainable Energy and Processes*. Perhaps an Energy Institute will be created in cooperation with other national players in this domain.

The Committee was impressed by the strength and quality of many of the programmes. It is worried about the embedding of the theoretical chemistry within the Inorganic chemistry group, which may undesirably reduce the availability or inclusion of theoretical methods by the other programmes. The Committee agrees with the choices made concerning the strengthening of research activities by the Sector Plan. However, it hopes that in the context of structural biology implementing a new and important research group, this would not lead to a decrease of funding to other parts of this area also in need of continuous infrastructure renewal, such as the Utrecht NMR facilities.

7B. PROGRAMME LEVEL – Utrecht University

Programme UU 1: **Biomolecular Mass Spectrometry and Proteomics**
Programme director: Prof. A.J.R. Heck
Research staff 2009: 28.9 fte

Assessments:		
	Quality:	5
	Productivity:	5
	Relevance:	5
	Viability:	4

The research programme in Biomolecular Mass Spectrometry and Proteomics focuses on the development of mass spectroscopic (MS) technologies for structural and functional analysis of proteins and proteoms. The activities include the employment of a combination of analytical chemistry, biochemistry and bioinformatics for proteomics technology development. Several research projects concern the proteomics of stem cells, chemical proteomics in cardiovascular diseases, drug interactions, and structural biology of folding processes, viruses and bacteriophages and transcription protein complexes. The programme emphasizes the method of mass spectrometry and its applications that are in a state of explosive development and of central importance for molecular life sciences. The programme is engaged in many different research collaborations within and outside Utrecht University.

Quality
This programme has contributed to important methodological innovations, which become standard for MS laboratories. The technology that they developed is used to tackle interesting questions in various fields, such as transcription regulation, stem cell biology and virology, in collaboration with international partners. The quality of research is excellent and the group is internationally highly competitive. The programme has succeeded in becoming one of the leading MS hubs in Europe with an excellent reputation, as judged by the numerous invitations for Prof. Heck to speak at top level conferences, prizes, and collaborations with leading laboratories and industry worldwide. The infrastructure and the funding situation of the group is excellent, which is a reflection of the strong leadership by Prof. Heck, who has managed to initiate and organise research programmes at both national and international levels, in which the UU 1 programme plays a central role.

Productivity
The productivity of this group is impressive, as judged by quantity and quality of the papers. A majority of the papers is published in the top 25% scientific journals. All metrics represent substantial and sustained improvements since 2001.

Relevance
The programme emphasizes the method of mass spectrometry and its application that is in a state of explosive development and of central importance for molecular life sciences and biomedicine. As a consequence the programme is engaged in many different national and international research collaborations in addition to those within Utrecht University. The programme's objectives are timely and well embedded in the Utrecht Campus.

Viability
The broad methodological scope and powerful range of mass spectroscopic experience in the group ensures depth and flexibility, and renders it well prepared for new scientific challenges. The

programme is well positioned for maintaining its role as a major player in the MS field internationally, and for sustained contributions to proteomics analyses in specific scientific fields, such as stem cell research. One apparent weakness is that despite its large size and methodological key role, this programme is headed by only one senior person (Prof. Heck) and has few permanent research staff. Furthermore, while the current equipment is state-of-the-art and sufficient, it is a vital issue to secure the development and maintenance of this important technology in view of the high obsolescence rate of MS instrumentation.

Conclusion

This group is one of the internationally leading groups in the field of biomolecular mass spectrometry and shows strong performance in methods development and proteomics of central biological processes. The group is internationally highly recognized and engaged in top level national and international collaborations. The Committee recognizes the excellent scientific output, which shows a clear upward development since 2001. The programme has all the necessary elements for a future continuation of its excellent scientific performance.

Programme UU 2: **Cellular Protein Chemistry**
Programme director: Prof. I. Braakman
Research staff 2009: 11.1 fte

Assessments:		
	Quality:	5
	Productivity:	4
	Relevance:	5
	Viability:	4

The research programme in Cellular Protein Chemistry addresses the molecular mechanisms of protein biogenesis and folding in eukaryotes. The programme employs a range of structural, biochemical and cell biological approaches to unravel principles and biomedical aspects of folding, conformational dynamics and quality control of resident proteins of the endoplasmic reticulum (ER), viral proteins, membrane proteins and molecular chaperones. This topic covers fundamental aspects of cell biology and biochemistry and has close links to protein folding diseases, such as cystic fibrosis (CFTR).

Quality
Although being one of the smallest programmes in the department, it has made major contributions towards central issues in the area of protein folding in the ER, including the mechanisms of co-translational folding of disulfide-bridged proteins (Prof. Braakman) and the identification of the ER origin of peroxisomes (Prof. Tabak). The group of Dr. Rüdiger has initiated an impressive tour de force approach to investigate structural features of the large, dimeric 90 kDa chaperone, Hsp90, by NMR. The programme leader Prof. I. Braakman is one of the world leading researchers in the field of protein folding with a very high international reputation. Prof. Braakman is organiser of and frequent speaker at international conferences.

Productivity
This programme has a continuously very good productivity of high quality publications, including papers in top ranked journals. The publications from all three PIs (Braakman, Rüdiger and Tabak) have the reputation of profound quality and are very well cited.

Relevance
The research of this programme addresses central questions of protein biochemistry and cell biology and has numerous biomedical implications, including the work on the molecular basis of cystic fibrosis, and the maturation of viral proteins of HIV and Influenza during the infection cycle. It is the declared aim of this programme to engage in biomedical research whenever the basic research activities provide a new lead.

Viability
The programme has strong links to other Utrecht chemistry programmes, notably the programme UU01 on Biomolecular Mass Spectrometry and Proteomics, UU06 on Biomolecular NMR Spectroscopy, and is furthermore embedded in collaborations with other programmes of Utrecht University and internationally with groups of leading scientists. The synergistic employment of structural biology, protein biochemistry and cell biology provide the required breadth and depth to achieve the ambitious goals. However, in order to ensure that the team can react to novel challenges and can maintain its competitiveness, the Committee finds it advisable that this relatively small programme acquires additional state-of-the-art approaches. To achieve this it is recommended to expand this programme by one additional junior group.

Conclusion

This is a very competitive and successful programme in the field of protein folding. The group is internationally highly recognized and publishes well cited papers of outstanding quality. The establishment of further collaborations with complementary groups and the development of novel approaches within the programme through an additional group would ensure the continued success of the programme.

Programme UU 3:	**Biological and Chemical Crystallography**	
Programme director:	Prof. P. Gros	(Protein Crystallography)
	Prof. A.L. Spek	(Chemical Crystallography)
Research staff 2009:	10.3 fte	

Assessments:	Quality:	5
	Productivity:	5
	Relevance:	5
	Viability:	4

An underlying emphasis of this research programme is the application of crystallographic methods, and the group is on the international forefront in both biological and chemical crystallography with valuable cross-fertilisation between the two fields, most recently in data analysis. The biological research addresses the most challenging biomedical questions, and has established an internationally leading position in preparation and structure determination of biomolecular complexes, a position that is supported by the available infrastructure. The chemical crystallography team holds an equally strong international position, due to the development of validation software used worldwide, the operation of the National Single crystal facility, and the expertise in determination of complex structures. The programme emphasizes fundamental understanding at the lead-edge in structural biology and chemistry, with particular focus on molecules involved in recognition events or regulation in biomedical processes.

Quality
The programme is comprised of an internationally leading group of researchers, whose work exhibits both depth and breadth. The team has an outstanding publication record that includes papers in top international journals during the review period. These publications contain many outstanding research results, among them Prof. Gros' work on the immune system. Team members' international recognition is illustrated by a large number of invited/ plenary/keynote international lectures and the receipt of numerous awards, which include the Trueblood Award to Prof. Spek and the Spinoza award to Prof. Gros.

Productivity
During the current review period, the research team has exhibited a high publication rate that includes high-quality publications in top-rated journals and three patents. Staff numbers have remained stable, while funding resources have doubled during the review period.

Relevance
This programme addresses fundamentally interesting and biochemically/biomedically important applications that are at the forefront of understanding complicated biomolecular and chemical compounds, theirs structures and functions. The programme trains students and post-docs in scientific fundamentals with valuable expertises in these areas that are in high demand. Strong research collaborations exist between this programme and large pharmaceutical companies. The programme oversees a service centre for conducting single-crystal measurements and analyses, which is an important national resource and provides fruitful opportunities for external collaborations; it is currently transforming to a fee-for-service operation that is intended to be self-sustaining.

Viability
The team's reputation and leadership in advancing the state-of-the-art crystallography in chemical and biological sciences place them in a position of strategic advantage for the future. Sustaining such excellence will require continued investment in developing the methodologies that give this

programme its competitive advantages. Strong collaborations exist with research partners at Utrecht University and at other Dutch or international institutions that provide complementary medical, biological, biochemical, or method development expertises. Future goals that focus on order-disorder phenomena could benefit from collaborative interactions with the strong solid-state NMR group of Prof. Marc Baldus in UU06.

Conclusion

The programme exhibits excellence and exceptionally high productivity of research. The activities span chemical and biological structure determinations and the expertise to produce the crystals, which provides the depth, breadth, and versatility to achieve the goal of the programme. The review committee draws attention to the need to continue investments that will allow the programme to maintain and lead development of infrastructure (including hardware, methodologies, and services), which pay dividends with respect to the programme's high international research profile and broader benefits to Dutch and international science.

Programme UU 4: **Medicinal Chemistry and Chemical Biology**
Programme director: Prof. R.M.J. Liskamp
Research staff 2009: 14.6 fte

Assessments:		
	Quality:	4
	Productivity:	4
	Relevance:	4
	Viability:	4

The objective of this programme is the design and synthesis of building blocks of peptidomimetics, dendrimers and scaffold molecules for influencing protein-protein and protein-carbohydrate interactions implicated in various biological processes and diseases. The programme is part component of the "Drug Discovery" research area and is a combined molecular effort in which structural, synthetic and (bio)physical chemistry approaches are integrated. The majority of the staff is funded by the Department of Pharmaceutical Sciences, and the group is heavily engaged in the teaching of pharmacy students.

Quality
The Medicinal Chemistry and Chemical Biology group has an active research programme characterized by the integrated employment of a broad spectrum of methods. In the past years the group has made significant progress in the development of novel tools for the chemical synthesis of dendrimers, the display of carbo-dendrimers of synthetic scaffolds, and the application of chemical biology for interfering e.g. with microbial growth, inflammation and amyloid formation. The programme has achieved a nationally leading position in its field, and Prof. Liskamp participates in several committees and editorial boards of international journals.

Productivity
The research activities of this programme have yielded a fairly large number of publications (relative to the group size) in international journals with an average citation record. Considering the relatively small staff number the number of defended Ph.D. theses is high.

Relevance
Medicinal Chemistry and Chemical Biology in general, and the scientific focus of this programme in particular, are of high societal relevance, since compounds may be generated that influence biological processes and disease states and hence are of profound importance for academic research and medical applications. Furthermore, the group has a good tradition of collaborations with companies. The fact that this group has filed 6 patents is a strong indicator of this link and of the success of this group in the application of their research.

Viability
The research field of this programme is optimally positioned for collaborations with various partners from different disciplines. This is reflected in a large number of existing collaborations within the Bijvoet Centre of the Department of Chemistry, the focus area "Drug Innovation" and many more laboratories and companies at the national and international level. The methodological broad range of this programme provides robustness and stability to the group. The scientific infrastructure available at UU is considered to be excellent, which is also stabilising. However, this programme frequently operates on the basis of only one PhD student per subject, with no possibility of extending the research beyond the PhD. This represents a strategic disadvantage (e.g. because it is difficult to maintain scientific knowhow in the lab) and efforts to improve this situation would be desirable.

Conclusion

The research carried out in this programme is highly relevant for industry and academic research. The achievements of this programme are very good. The future potential of this programme is high since there will be continuous need for chemical tools to interfere with biological processes and disease states. It will be critical to integrate the various team members into a coherent research programme which generates synergisms and secures the methodological knowhow in the group.

Programme UU 5: **Membrane Enzymology**
Programme director: Prof. G.F.B.P. van Meer
Research staff 2009: 10.5 fte

Assessments:		
	Quality:	5
	Productivity:	4
	Relevance:	5
	Viability:	5

The objective of this programme initiated in 2001 is the elucidation of the regulatory mechanisms of membrane lipid homeostasis, the physico-chemical properties of membrane lipids in relation to their cellular functions, and the application of the acquired insights for translational research. This is field of research is highly relevant both for basic science and biomedicine, and offers great perspectives since even fundamental issues remain to be worked out.

Quality
During the review period the programme has produced numerous important scientific highlights, among which the discovery of mechanisms to generate and transport sphingolipids, the identification of roles for glycolipids in protein sorting and function, the dissection of the role of flippases in vesicle formation, the discovery of a novel family of integral membrane proteins acting as sphingomyelin synthases, and the elucidation of principles of the regulation of lipid homeostasis. The academic reputation and scientific leadership by Prof. Van Meer and the other members of the group are excellent, as judged by numerous collaborations with top groups worldwide, the coordination functions in 3 EU networks, the organisation of high level international conferences, awards, functions in important committees and Editorial Boards of major journals (Prof. Van Meer), and many invitations to international conferences. This innovative programme holds a strong international position with great perspectives in the future.

Productivity
Since 2001 this programme has continuously increased the number and impact of publications and has at the end of the period reached a high productivity. All PIs of this programme have a good track record with high impact publications and invitations to conferences. Moreover the group has a total of 18 patent applications since 2001, showing the strength of this programme at the intersection between basic and translational research.

Relevance
The research topic is tightly linked to the molecular basis of disease and the programme has put major emphasis on the translation of their results into medical applications. This is underscored by the high number of patent applications, the organisation of high level workshops (EU wide) where the medical applications are covered and the chairing of the ESF expert group to establish the ESF policy regarding the importance of lipidomics for health and disease (Prof. van Meer).

Vitality
The research area of this programme offers a rich field of unsolved questions of fundamental importance for understanding membrane function and regulation. The research activities are based on a powerful combination of approaches ranging from lipid and protein chemistry to cell biology and genetics. Furthermore, the programme is engaged in numerous fruitful collaborations and takes active steps towards the re-organisation of groups within the UU Campus, to generate closer links and a communicative environment between the relevant laboratories. The Committee considers this to be an important step in the right direction. Overall this programme is in a strong position to contribute to significant discoveries in the future.

Conclusion

This research programme is full of life and productivity and has made impressive achievements since its start in 2001. Its multidisciplinarity, the participation in local and international research networks and the strong leadership renders this programme highly competitive and well prepared for future scientific challenges.

Programme UU 6:	**NMR Spectroscopy**	
Programme director:	Prof. M. Baldus	Biomolecular solid-state NMR (from August 2008)
	Prof. R. Boelens	Biomolecular solution-state NMR
	Prof. A. Bonvin	Computational structural biology
Research staff 2009:	22.6 fte	

Assessments:	Quality:	5
	Productivity:	4
	Relevance:	5
	Viability:	5

The NMR spectroscopy programme is engaged in the development and application of new methods for analysis of the structures and dynamics of protein-DNA complexes in transcription and DNA repair, photosensory proteins and ubiquitination complexes. It combines solution- and solid-state NMR spectroscopy and integrates these approaches with molecular biology and computational structural biology.

Quality
This is an excellent team of researchers pursuing leading-edge understanding of biomolecular structure and function. The expertises of Prof. Boelens and recently retired Prof. Kaptein in solution-state NMR, Baldus in solid-state NMR, and Bonvin in computational structural biology are complementary, and at a top international level. Collaborations between experimentalists and theoreticians appear strong and effective. The scientific highlights, elucidating the structures and dynamics of complex multi-component systems are impressive. The quality of these studies and their impact are generally excellent. The international reputation of the group leaders is high, as evidenced by numerous invitations to participate in and organize international conferences, prestigious prizes and editorial board memberships. This group hosts the leading central infrastructure of an open EU-NMR network. The funding situation of this programme is therefore excellent and includes several large EU grants.

Productivity
The publication record of this programme is very good. Structural biology of this type does not lead to a large number of publications, but this group publishes in top journals and has had high impact.

Relevance
The research themes of this group have strong links to biomedicine since the structures under investigation relate to DNA repair and mechanisms of antibiotics. Furthermore, the computational programmes developed to predict protein interactions may be useful for the identification of drug targets. The research themes being pursued are motivated by important biochemical, biological, medical, or biotechnological applications. The NMR expertises of this programme are highly valuable for other research activities in Utrecht and elsewhere.

Vitality
With the existing professorships for solution-state NMR, solid-state NMR and computational structural biology, and the embedding in the department of Chemistry that also offers X-ray, mass spectrometry and biochemistry, this programme offers a broad scope and ideal combination of methods. The appointment of Prof. Baldus has significantly expanded the scope the programme to include solid-state NMR with a view to understanding proteins in membrane environments and poorly ordered aggregates such as amyloid plaques. The programme is well led

by a young team. One concern is that there must be sufficient sustained funding for the technical and scientific support of the NMR instrumentation that will be required to maintain the programme's strong international profile.

Conclusion

This research programme displays vitality and competitiveness at the international level. It plays a major role in national and international NMR networks.

Programme UU 7: **Biochemistry of Membranes**
Programme director: Prof. J.A. Killian
Research staff 2009: 8.4 fte

Assessments:		
	Quality:	4
	Productivity:	4
	Relevance:	4
	Viability:	4

The research of this programme aims at understanding the organisation, structure and function of membranes at a molecular level and developing chemical approaches to manipulate membranes. It integrates membrane biochemistry, chemical biology, biophysics, structural biology and molecular genetics.

Quality
The Biochemistry of Membranes programme has generated interesting results concerning the development of nanocapsules for the efficient delivery of drugs, the mechanism of the peptide antibiotic nisin, the further development of model systems for the analysis of protein-lipid interactions, and the determination of effects of amyloids on membrane integrity. The academic reputation of this programme is very good and has led to several international collaborations. The programme shows a coherent scientific output, but the retirement of Prof. De Kruijff and successive reorganisations have left a gap not yet fully filled by Profs. Killian and Breukink in terms of recognition, citation, group size and grant income.

Productivity
Productivity dropped substantially during the review period but has recovered in recent years. Significant results on nanocapsules and nisin mechanism were published in very good to excellent journals.

Relevance
The nanocapsules and the work on the antibiotics have clear relevance for medical application. Future work is needed to develop these novel findings for applications. The relationship between the academic programme and spin-out QVQ is unclear.

Viability
The group is rather small and appears to have had difficulties in maintaining the critical mass of infrastructure and scientific know how. The Committee has been informed of a planned merger of this programme with the programme UU05 Membrane Enzymology, a step that has been endorsed by both partners of the merger. We consider this as scientifically reasonable and hope that the successful merger will stabilize and strengthen the research of this programme in the future.

Conclusion
The research carried out in this programme is positioned at the intersection between basic and applied membrane science. In response to changes related to the retirement of the former programme leader Prof. B. de Kruijff, and with the aim of improving the international competitiveness of membrane research at UU, a merger of this rather small programme with the scientifically complementary programme UU05 under the leadership of Prof. Van Meer is planned. The Committee considers this to be an ideal solution.

Programme UU 8:	**Organic Chemistry and Catalysis**	
Programme director:	Prof. R.J.M. Klein Gebbink	Homogenous and bioinspired catalysis
	Prof. L.W. Jenneskens	Physical organic chemistry
Research staff 2009:	10.7 fte	

Assessments:	Quality:	4
	Productivity:	4
	Relevance:	5
	Viability:	4

The focus is on syntheses of organic molecules, principally via homogeneous catalysis and with inspiration from biology. The programme is developing a vibrant pursuit of projects in new areas, reducing the emphasis on traditional organic synthesis methodologies. The programme is adjusting to the retirement of Professor Van Koten and other organizational changes implemented during the review period.

Quality
This programme consists of a vibrant group of researchers that are pursuing fundamental scientific understanding of solution-phase catalysts. The team has published high quality papers in top international journals during the review period. Prof. Van Koten, who has been a major international leader for many years, retired midway through the review period, though he remains affiliated with the programme. His successor, Prof. Klein Gebbink, appears very promising but has yet to fully establish himself as a major independent personality, while Prof. Jenneskens now publishes very little.

Productivity
The team has had publications in high-quality journals, including several in top chemistry venues and six patents. There has been a strong and continuous flow of high quality publications despite 50% reductions in research funding and staff.

Relevance
The programme's objectives are timely and societally important, addressing energy sustainability, environmental, and organic/biochemistry fundamentals and applications in which students are broadly trained. Substantial direct support has been obtained from industrial sponsors for a number of projects. These, and the patent applications produced during the review period, manifest a strong connection between basic science and technology. The focus on homogeneous catalysis is complementary to other Utrecht programmes, with mutually valuable collaborations with the heterogeneous catalysis groups of Prof. De Jong and Prof. Weckhuysen (UU10), the Debye Institute of Nanomaterials, and Utrecht's Chemical Biology Programme and Medical Centre.

Viability
Strong expertise in organic synthesis, homogeneous catalysis, and computation underpins the programme, but the apparent absence of a strong organic-synthesis-methodology effort leaves it vulnerable to losing important training skills for students, as well as missing sources of new research directions and opportunities. The absence of junior faculty members means that the group is in danger of being sub-critical in size and range of expertise, threatening its long-term viability. In addition, characterization activities appear to be relatively standard: there could be a greater emphasis on the use of advanced characterization techniques for understanding and bridging the synthesis and computational strengths of the team. The strengths of the NMR and vibrational spectroscopy groups represent opportunities for mutually beneficial cooperation.

Conclusion

The programme appears to be stabilizing after a transitional period of reorganization, but may currently be too small to remain seriously competitive internationally. Prof. Klein Gebbink projects strong leadership skills that will benefit the programme and its future. The team should consider keeping a strong synthesis-methodology component within its activities, along with augmenting its characterization pursuits, especially to take advantage of the powerful spectroscopy resources and capabilities available collaboratively within adjacent chemistry programmes.

Programme UU 9:	**Condensed Matter and Interfaces**	
Programme director:	Prof. A. Meijerink	Solid state chemistry
	Prof. D. Vanmaekelbergh	Chemistry and physics of nanostructures
Research staff 2009:	14.1 fte	

Assessments:	Quality:	5
	Productivity:	5
	Relevance:	5
	Viability:	4

The research programme in Condensed Matter and Interfaces emphasizes nanostructured opto-electronic materials, especially semiconductor nanocrystals and related systems where quantum confinement effects may be important. This programme is fundamental in scope, providing understanding that is directed to numerous potential uses in sustainable energy, energy efficiency, and medical imaging applications. Its activities span the syntheses and characterization of the structural, optical, and electrical properties of nanoscale materials and their associated applications.

Quality
This is an internationally leading programme that is advancing fundamental knowledge, properties, and methodologies of synthesis and characterization of solids, especially those where interfaces are important. The team has published high quality papers in top international journals during the review period. Team members have presented a large number of invited/plenary/keynote lectures and are editors or editorial board members of two technical journals in their field. They have received numerous recognitions, including the Centennial Award of the Electrochemical Society and the recent election of Prof. Meijerink to the Royal Netherlands Academy of Sciences.

Productivity
This team has an excellent publication record, with numerous highly visible and highly cited papers in top-rated journals and several patents.

Relevance
The programme's technical objectives are timely and societally important. Training of students is broad and interdisciplinary across the fields of chemistry, physics, and materials science. The focus on luminescent or opto-electronic materials is complementary to other Utrecht chemistry programmes, notably the inorganic chemistry and heterogeneous catalysis pursuits in UU10. There has been significant growth (a near doubling) of funding resources during the review period, with staff increasing by 25%. This reflects the programme's importance for energy conversion and efficiency, its associated societal importance, and commercial promise. The latter is evidenced by the team's six patent applications produced during the review period.

Viability
This is a powerful team that is well placed to continue its high quality and innovative work. The fundamental focus and strong spectroscopic/imaging capabilities yield general understanding that can be adapted or transferred to related systems, for example nanostructured metals or metal oxides used in catalysis (UU10), or to soft-condensed matter systems. The field of nanostructured luminescent/opto-electronic materials is rather crowded, and competition will remain fierce. To stay at the leading edge in this area will require agility and vigilant maintenance of the

programme's competitive advantages in the development of new synthesis, characterization, and modelling methodologies.

Conclusion

The programme is at a top international level in the field of nanostructured semiconductor materials. It integrates preparatory chemistry and processing with property measurements aimed at advancing the understanding of these complex heterogeneous systems. Maintaining the team's high profile in this highly competitive field will require agility and sustained efforts. Integration of the theoretical chemistry group (UU12) provides an opportunity to augment the cooperation between the programme's strong experimental pursuits and property modelling. In addition, fostering closer ties with industry could assist the team with targeting important technologically problems, and to provide opportunities for following up commercially promising discoveries.

Programme UU 10:	**Inorganic Chemistry and Catalysis**	
Programme director:	Prof. K.P. de Jong	Synthesis of catalysts and sorbents
	Prof. B.M. Weckhuysen	Spectroscopy of catalyst materials at work
Research staff 2009:	36.8 fte	

Assessments:	Quality:	5
	Productivity:	5
	Relevance:	5
	Viability:	5

The research programme in Inorganic Chemistry and Catalysis is focused on the development and understanding of heterogeneous inorganic systems for promoting heterogeneous chemical reactions. The scope of activities includes design, syntheses, characterization and applications of catalysts that cover molecular to macroscopic length and time scales. The programme emphasizes fundamental understanding of complex catalytic materials for reactions that are of industrial or societal importance in energy or environmental applications.

Quality
This programme engages an internationally dominant group of researchers that are pursuing leading-edge fundamental scientific understanding of catalysts of high technological importance. The programme takes advantage of the team's international leadership in powerful characterization techniques, Prof. de Jong's in three-dimensional electron microscopy/tomography and Prof. Weckhuysen's in in-situ spectroscopy, and correlates them directly with catalyst preparation and function. The team has published many excellent papers in top international journals during the review period .The team members have presented a large number of invited/plenary/keynote lectures, are on the editorial boards of several technical journals in their field, and have received numerous award recognitions.

Productivity
This team has an excellent publication record with numerous highly visible papers in top-rated journals, 12 patents, and several books written or edited by senior faculty. There has been significant growth (more than doubling) of funding resources during the review period. All metrics represent substantial and sustained improvements since 2001.

Relevance
Inorganic chemistry and catalysis are central to important energy and environmental applications that are crucial to society. This is manifested by strong research funding from industrial sponsors, strong job prospects for graduating students, and the patent applications produced during the review period. The programme's objectives are timely and important, providing both broad and deep training to students in scientific fundamentals and their uses in energy and environmental contexts. The focus on heterogeneous catalysis is complementary to other Utrecht chemistry programmes, notably the homogeneous catalysis pursuits in UU08 and nanostructured semiconductors in UU09.

Viability
The strong links between catalysts synthesis, characterization, and applications ensure depth, breadth, and versatility to achieve the goals of this programme. The fundamental focus yields general understanding that can be adapted or transferred to related systems, allowing the team to be responsive to new opportunities or changes in priorities. The key strengths of the programme that should be sustained by appropriate investments are the ability to develop and to have access

to state-of-the-art characterization instrumentation and techniques. Several of these are at the top international level and/or are unique in the Netherlands. Incorporation of more theoretical activities alongside the excellent synthesis and characterization capabilities would further enhance the scope of this excellent programme.

Conclusion

The programme is among the very top internationally in the field of heterogeneous catalysis, combining powerful and collaborative expertise in synthetic inorganic chemistry, characterization, and reaction testing. Continued collaboration with related programmes in homogeneous catalysis and industry, in addition to augmenting theoretical activities, will further promote the strengths and synergies of this strong programme.

Programme UU 11:	**Physical and Colloid Chemistry**	
Programme director:	Prof. W.K. Kegel	Self-organizing systems
	Prof. H.N.W. Lekkerkerker	Physical chemistry
	Prof. A.P. Philipse	Colloid chemistry
Research staff 2009:	18.7 fte	

Assessments:	Quality:	5
	Productivity:	4
	Relevance:	5
	Viability:	4

The research programme in Physical and Colloid Chemistry is focused on the characterization, understanding, and properties of assemblies of solid colloidal particles. The scope of activities includes principally synthesis, structural characterization and understanding physical phenomena associated with colloidal assemblies, particularly using scattering and imaging analyses.

Quality
The researchers in this programme have strong reputation in experimental physical analysis of colloidal systems. The scope of their research emphasis is fundamental and involves systems with numerous potential applications. The team has published many excellent papers in top international journals during the review period. Prof. Lekkerkerker in particular was recognized with international awards from the European Physical Society and the European Colloid and Interface Society. Collaborations with computational and theory groups augment the experimental strengths of the team.

Productivity
The team is productive and collaborative with numerous publications in top-rated journals as stated above. The publication rate remained approximately constant (ca. 30 papers per year) although funding and staffing increased during the review period. Two patents were filed during this time.

Relevance
This programme is focused predominantly on the packing structures and dynamics of colloidal solids of diverse composition and under various conditions (density, external fields). The team's emphasis is concentrated on understanding the fundamental physics of solid colloidal systems, which are ubiquitous in nature. Soft colloid systems are not featured strongly in the programme, although recently solid-stabilized emulsions have been investigated and progress in theory and simulations of soft condensed systems were mentioned. Connections to applications were not explained in detail but appear to include collaborations with industry and research supported by industry (e.g., Schlumberger, Shell, Unilever).

Viability
Strong expertise in scattering (X-rays and neutrons) and microscopy underpin the efforts of this group. The fundamental focus yields general understanding that can be adapted or transferred to related systems. Much use is made of international X-ray scattering facilities, especially the European Synchrotron Radiation Facility. Relatively conventional chemical syntheses appear to be undertaken in-house, but synthetic activities in the programme could be more strongly emphasized. Computational modelling efforts were also mentioned, but were not featured prominently in the written or oral review summaries. Augmenting the research expertises of the team in the areas of synthesis and computational modelling of colloidal systems could open new

opportunities and enhance the programme's scope, versatility, and impact. The forthcoming retirement of Prof. Lekkerkerker early in the next review period means that the group will face a transition of leadership with respect to its organization and pursuits, and this presents both opportunities and uncertainties.

Conclusion

The strong publication record during the recent review period reflects a dynamic, collaborative, and internationally leading scientific programme. Excellent use is made of international experimental facilities, which enable state-of-the-art scattering measurements and analyses by the team. Synthesis and computational modelling efforts did not feature prominently in either the written or the oral summaries and appear to have conspicuously low priorities in the programme. The programme's focus on solid colloidal systems could be extended to include more soft colloidal systems. Looking to the future, the review committee is concerned whether the programme will be able to maintain its current strength following Prof. Lekkerkerker's retirement.

Programme UU 12: **Theoretical Chemistry**
Programme director: Dr. J.H. van Lenthe
Research staff 2009: 1.4 fte

Assessments:	Quality:	no score
	Productivity:	no score
	Relevance:	no score
	Viability:	no score

This programme will be discontinued and brought into UU 9.

The group strives to develop methods to compute huge molecules or molecules containing heavy metals. Also, parallel approaches are developed, allowing Ab Initio electronic structure calculations with over 7000 atoms. This finds applications in Computer Aided Drug Design. The development of relativistic methods facilitates heavy metal chemistry. The programme has been drastically downsized with respect to funding and staff (< 2 FTEs) during the review period and will be discontinued and folded into UU 9.

Quality
This programme was internationally visible. It was focused on the development of computational methods for large molecules, molecules containing heavy atoms, model analyses, and massively parallel strategies for calculating electronic structures of large ensembles of atoms. The review committee was impressed by the commitment of Dr. van Lenthe to his scientific work and to his students, despite the major structural changes that were imposed and his own difficult health circumstances.

Productivity
Quality publications appeared early in the review period in highly rated chemistry and physics journals, and team members presented a large number of invited lectures. However, the downsizing resulted in drastic drop in papers published yearly, with only two in 2009, which is low even taking into account the reduced resources and staff available. Anxieties about the future and organizational instability have undoubtedly contributed to a difficult work environment and low morale.

Relevance
Theoretical chemistry is a crucial fundamental research area that touches on all aspects of chemistry and its applications. It provides important fundamental skills and insights across numerous chemistry, physics, materials science, and engineering disciplines. The training of students in theoretical chemistry is important and should be fostered, especially alongside experimental chemistry programmes, where substantial scientific synergies exist.

Viability
The current programme is being phased out and has been below critical thresholds of funding and staffing during much of the review period.

Conclusion
The review committee emphasizes the importance of maintaining strong theoretical components within the chemistry department at Utrecht. The Committee urges that adequate resources (funding and staff) be provided to bolster theoretical activities within the appropriate chemistry programmes (e.g., UU 9, but also others), all of which would likely benefit from synergy between experimental and theoretical pursuits.

8A. INSTITUTE LEVEL – VU University Amsterdam

University: VU University Amsterdam
Faculty: Faculty of Sciences
Department: Department of Chemistry and Pharmaceutical Sciences
Institutes: Amsterdam Institute for Molecules, Medicines and Systems (AIMMS)
Amsterdam Center for Multiscale Modeling (ACMM)
Amsterdam Institute for Lasers, Life and Biophotonics (LaserLAB Amsterdam)

1. Structure

The Faculty of Sciences (FoS) offers research and education in the natural sciences, mathematics and computer science. The research of FoS is organized in four Departments: Computer Sciences, Physics & Astronomy, Chemistry & Pharmaceutical Sciences, and Mathematics. FoS participates in five interdisciplinary interfaculty research institutes: the Network Institute, Neuroscience Campus Amsterdam, the Institute for Lasers, Life and Biophotonics (LaserLAB Amsterdam), the Amsterdam Institute for Molecules, Medicines and Systems (AIMMS) and the Center for Advanced Media Research Institute (CaMeRa). FoS is also involved in various research schools and national institutes.

The Department of Chemistry and Pharmaceutical Sciences aims to advance the Molecular Sciences and to educate curious and creative scientific professionals for the benefit of society. The Department strives to be an internationally leading research institute, performing cutting-edge research on molecular systems, biomolecular interactions and their applications in the Health and Life Sciences.

The research activities of the eleven chairs of the Department are organized in six research programmes that are subject of this review. All research areas of the department are embedded in two major research themes of the VU University: *Human Health & Life Sciences* and *Energy & Sustainability*.

Since 2005 the Department has organized its Chemistry research around three major research areas

- Molecular Pharmaceutical Sciences/Synthesis in Life Science Chemistry
- Computational Chemistry
- Analytical Chemistry & Spectroscopy.

Since April 2010 these research areas are embedded in three multidisciplinary, interfaculty and inter-university research institutes:

- ***Amsterdam Institute for Molecules, Medicines and Systems***

The mission of AIMMS is to join forces in basic molecular Life Sciences to reach fundamental breakthroughs in translational molecular medicine with emphasis on the integrated understanding of biological processes and systems and the development of new drugs, therapeutics and diagnostics. The research focuses on the fundamental understanding of biological processes from molecules to networks. AIMMS integrates chemical, pharmaceutical, biological and related medical sciences at the VU.

- ***Amsterdam Institute for Lasers, Life And Biophotonics***

The mission of the LaserLAB Amsterdam is to perform research using the interaction of (laser) light and matter on systems ranging from atoms and molecules to living cells and tissue. A recent focus within LaserLAB is on the further development of new methods and techniques, new equipment and tools, to study fundamental aspects of living systems to provide novel medical diagnostics and clinical treatments. LaserLAB will forge close interaction and collaboration with VUmc and AMC and will develop a new Master programme that will be profiling Laser Sciences at the national and international level.

- ***Amsterdam Center for Multiscale Modeling***

The aim of ACMM is to develop computational tools to model and predict the behaviour of complex chemical and biological processes, to collaborate with users in industry and academia in order to apply these tools to problems of great societal relevance, and to disseminate the knowledge about multiscale modeling by training through national and European training courses for students and research scientists.
Three groups form the ACMM core: (1) Division of Theoretical Chemistry, VU, (2) Computational Chemistry and Physics, UvA, (3) Theoretical Biophysics, FOM Institute for Atomic and Molecular Physics. Other ACMM partners are Computational Biophysics (UT) and Organic Chemistry (VU).

The PhD-training is primarily organized through the two research schools HRSMC and LACDR. The scientific staff of the Department has a heavy teaching load in four BSc- and four MSc-programmes.

2. Societal Relevance

The research and teaching of the Department addresses key issues in society. The involvement in the VU central research theme Human Health and Life Sciences illustrates the commitment to significantly contribute to the diagnosis and therapy of diseases. The work in the field of catalysis and synthetic chemistry is directed towards Sustainability and Energy, with potentially a huge societal impact. The Department is a founder of the BSc/MSc programme Science, Business & Innovation, focusing on the translation of scientific knowledge into practical innovations that find their way into the business environment and into society in general.

The Department has a number of spin-out companies, such as SCM, IOTA and Griffin Pharmaceuticals. Some programmes have a very active policy with regard to building an IP-portfolio, often with support of the Technology-Transfer-Office of the VU. The Department anticipates that in the future the scientific staff will be more active and successful with regard to valorization, as staff becomes involved in the BSc/MSc programme Science, Business and Innovation (SBI).

3. Strategy for the future

In 2005, the Department, together with FoS, initiated a reorganization plan to refocus its resources on research themes with sufficient critical mass to be successful in both national and international competition, together with a budget reduction of about 20%. More recently, the Amsterdam Chemistry and Physics Departments have combined their research efforts in order to create focus and mass in areas of proven excellence. In these key research areas, the two Science faculties joined forces with many Amsterdam science partners from FOM/NWO institutes (CWI, AMOLF, NIHKEF) and the medical centres (AMC, VUmc, NKI) in what is called *Amsterdam: City of Science*.

The Department believes that the coordination between different Faculties within the VU and between two Universities (VU and UvA) will significantly strengthen the Department. The two Chemistry Departments of VU and UvA have aligned their research strategy. The VU focuses strongly on the area Chemistry of Life & Health. Combined VU-UvA efforts are especially in Theoretical Chemistry and Analytical Chemistry & Spectroscopy. In other areas the activities of both universities are complementary, avoiding duplication.

The Department has obtained support for the creation of new research chairs in Biomolecular Spectroscopy and Biocomputational Chemistry and the strengthening of recently created chairs by the appointment of assistant professors. With the appointment of five new professors in the recent four years and with two professorships to be created in 2011, the Department has undergone the necessary renewal to be competitive in a fast changing research world.

The Committee welcomes the stronger interaction with the UVA leading to a much better critical mass in a number of key areas. In particular a strong collaboration between the Spectroscopy group, strengthened by the Sector plan endowed Biomolecular spectroscopy chair and the Molecular photonics group of UVA in the context of the Laser Lab could make Amsterdam a leading centre of spectroscopy and photosciences .The collaboration of the computational groups of both universities would also make a broad and strong theoretical knowledge base further strengthening the already leading position in area of scientific activity that elsewhere in the Netherlands seems to be shrinking in activity.

8B. PROGRAMME LEVEL – VU University Amsterdam

Programme VU 1:	**Biomolecular Analysis and Spectroscopy**	
Programme director:	Prof. H. Irth	Biomolecular Analysis (BMA)
	Prof. C. Gooijer	Biomolecular Spectroscopy (BMS)
Research staff 2009:	10.5 fte	

Assessments:	Quality:	3
	Productivity:	4
	Relevance:	5
	Viability:	4

The mission of these groups is to develop and apply analytical methodologies for the discovery, structural characterization and trace level quantitation of biologically active molecules. A common theme in the research programmes is the integration of analytical techniques and instruments with methodologies from adjacent disciplines such as biochemistry, pharmacology, organic chemistry or physical chemistry in order to significantly enhance the information content of analytical methods. Research themes in BMA are Discovery Technologies and Hyphenated Analytical Technologies, while the research themes in BMS, are Bioanalytical Spectroscopy and Biophysical Spectroscopy.

Quality
The group is engaged in translational and enabling bioanalytical research. A key feature of the BMA programme is use of on-line technologies for the separation and selective detection and simultaneous quantification of mass and biological activity of compounds in complex mixtures, to facilitate discriminative high throughput screening in drug discovery. Additionally, research is directed to hyphenated ultrasensitive technologies, some involving discovery of new tagging agents, which are being developed for application to analysis of safety and activity biomarkers (proteins, small molecular weight compounds), and catalysts. The BMS programme is exploiting known (Raman and cavity ring down) spectroscopic and electrochemical properties of compounds in some innovative ways. Publications are consistently in good to excellent journals in analytical chemistry. It is an active local and national player, although interaction within the group appears modest, as implied by minimal joint publications. International recognition of its published output is good for BMA but appears limited for BMS. There is limited evidence of specific high-level international awards. PhD-student numbers have been high although the drift downwards over the review period is of concern. Student progress is good. Direct funding by the department has remained high. There is a sustained, reasonably healthy and balanced level of national external funding per fte with some recent EU funding. The research facilities are well used by scientists throughout Europe. The virtual absence of non-tenured research staff is noticeable.

Productivity
The number of refereed international publications per fte is reasonable, although slightly declining in recent years. The major administrative roles taken by Professor Irth have undoubtedly had an impact both on the productivity and on the visibility of the group's work.

Relevance
The relevance of the research topics to the solution of existing problems in the biological and biomedical arena is very high. Skilled, well trained graduates in analytical chemistry are in great demand nationally in many industries. Part of this demand is met by the provision of the only analytical chemistry M.Sc. degree in a chemistry department nationally. The development of

hyphenated technologies and of specific and sensitive methods of detection could greatly assist those working in the discovery of bioactive molecules. There is clear interaction with national institutions and with the main user of the group's technologies, the biopharmaceutical industry, which could be beneficially improved further. The IP surrounding the technologies developed is clearly exploitable.

Viability

The group has some difficulty in manning and maintaining its substantial instrumentation, although overall it is well resourced with state-of-the-art facilities. Increasing collaboration with its sister group at UvA, and its participation in the recently implemented joint universities AIMMS and LaserLAB Amsterdam should assure the strong future viability of the discipline if seriously pursued. Two new assistant professors have been recently recruited to the group, but the heavy administrative load on Professor Irth, and impending retirement in the next few years of Professor Gooijer are of concern regarding the senior leadership of the group, and will need attention.

Conclusion

The group currently has a strong presence in analytical chemistry, but urgent attention is required, in concert with UvA, to its future development, leadership and support if it is to fulfil its important academic and practical potential.

Programme VU 2:	**Medicinal Chemistry**	
Programme director:	Prof. R. Leurs (Oct 2002-2009)	Medicinal Chemistry
	Prof. H. Timmerman (2001-Oct 2002)	Medicinal Chemistry
	Prof. M.J. Smit (2006-2009)	Target and Systems Biochemistry
Research staff 2009:	22.4 fte	

Assessments:	Quality:	5
	Productivity:	4
	Relevance:	5
	Viability:	5

The Medicinal Chemistry programme is at the interface of chemistry and biology with the objective to understand ligand-protein interaction at the molecular detail, elucidate subsequent biochemical signaling networks and to use this knowledge for the computational design and synthesis of new bioactive molecules. The focus is target proteins and their interactions with biologically active molecules, combining biochemistry, computational modeling as well as the design and synthesis of novel molecules. Research is focused on two complementary themes, G Protein Coupled Receptors (GPCRs) and Fragment Based Drug Design (FBDD).

Quality
This is a well-structured innovative group, at the leading edge of its field and successfully building on a traditional international reputation for work on the structure and function of histamine receptors. The research is appropriately focused and the group has an excellent international reputation at the front of research both on G-protein coupled receptors and fragment based drug design. The laboratory profits from strong leadership, with a realistic view of its present and future capabilities. The group has an appropriate mix of competencies, a critical mass and high earning power.

Productivity
The programme has a very good track record in terms of the number of papers and citations. The current staff of the newly formed group has reached a very good level of scientific output in terms of publications, patents and Ph.D. theses.

Relevance
The societal relevance is strong, as the programme contributes to the validation of novel therapeutic targets and the identification of new drug candidates. The impact is materialized in the education of highly qualified scientists and creation of start-up companies and health. There strong links also on educational aspects with the pharmaceutical industry in particular through TI- Pharma. There have been conspicuous successes in developing useful compound tools for the industry to discover new drugs affecting the action of GPCRs. The group has responded in an innovative way to the wave of Fragment Based Drug Design and is efficiently surfing on it.

Viability
The transition of leadership from Prof. H Timmerman to Prof. R Leurs has worked very well. The new team has a good mix of competencies and their synergy is excellent and efficient. Staff, funding and publications are all in progress. The strategy to develop along two complementary streams with continuing research on the topology and function of GPCRs and a new programme on Fragment Based Drug Design is relevant and sound. To ensure what looks like a bright future, the necessary laboratory space should be available.

Conclusion

The Medical Chemistry programme is excellent and at the forefront of the GPCR drugs and Fragment Based Drug Design. The productivity is very good and the societal relevance is guaranteed through close ties to the pharmaceutical industry.

Programme VU 3: **Molecular and Computational Toxicology**
Programme director: Prof. N.P.E. Vermeulen
Research staff 2009: 10.9 fte

Assessments:		
	Quality:	4
	Productivity:	4
	Relevance:	5
	Viability:	5

The objective of the research programme in Molecular and Computational Toxicology is to elucidate the molecular mechanisms involved in drug disposition and drug toxicity, and use this knowledge in the drug discovery, development and safety. The group employs computational methods and experimental studies to understand the interplay between drug metabolism and toxicity in an application driven research programme. The programme is handled by three research teams possessing different expertise, in molecular toxicology, computational chemistry and toxicology, and in experimental cellular stress biomarkers and predictive safety biomarkers.

Quality
The group is well established and carries out very good research with a high impact relative to the average for the field, in which it has a pre-eminent international position. The research is of high interest both to basic research and for industrial applications. The very good position of the programme is indicated by the strong position within national and European funding (e.g. through TI Pharma and the IMI initiative). The group possesses the expertise, infrastructure and strong leadership to get on the international forefront of molecular toxicology.

Productivity
The productivity is very good. The laboratory has a very good track record with high quality output in the best journals of the discipline. The team leaders are very good, but they are also taking more and more global teaching and managerial responsibilities, which may affect the productivity.

Relevance
The laboratory has a leading position in predictive toxicology, one of the major fields of interest of the pharmaceutical industry. The societal impact is obvious as the tools developed by the group should allow acceleration and rationalization of drug development and production. Predictive toxicology is also of prime importance in system biology research in order to develop relevant pharmacological molecular probes. In addition, the partnership with industry seems to increase. This opens new perspectives but could also influence the productivity of the group.

Viability
The biggest challenge faced by the group it to maintain and improve their quality and productivity by integration of its different research components, while dealing with teaching and managerial responsibilities. It is also important to reach a balance between academic and contract research. It is well-placed to take advantage of the move in toxicology from animal models towards more *in silico* prediction based on 'humanised' in vitro systems. The synergy between the three different components of the programme could be reinforced around transversal projects. It is also important that the group continues to extend its external collaborations to marry its expertise at the molecular level with an understanding of more complex integrated cellular and in vivo systems.

Conclusion

The Molecular and Toxicology group is carrying out a very good and productive research programme. The results produced are very relevant to both academia and industry.

Programme VU 4:	**Organic Chemistry**	
Programme director:	Prof. K. Lammertsma	Organic and Organometallic Chemistry
	Prof. R.V.A. Orru	Synthetic and BioOrganic Chemistry (2007-2009)
Research staff 2009:	14.5 fte	

Assessments:	Quality:	4
	Productivity:	5
	Relevance:	4
	Viability:	5

The Organic Chemistry group focuses on the design of new reactions that minimize both energy consumption and chemical waste production but at the same time open new regions of chemical space. OOC explores new chemistry that focuses on the sustainability of phosphorus, including recycling current waste organophosphorus products, catalytic reactions that eliminate organophosphorus waste, transition metal complexes with low valent phosphorus ligands, and sustainable building blocks, polydentate ligands and catalysts. The main research programmes of the SBC group are the design, development and exploration of new multicomponent reactions (MCRs) for atom- and step-efficient synthesis, including asymmetric methodology employing transition metal-, organo- and biocatalysts, and the design of small molecular probes for applications in chemical biology, medicinal chemistry, catalysis and material research.

Quality
The Division consists of two very good research groups. The OOC group is well established, playing a significant role in organophosphorous chemistry worldwide. The SBC Group is more junior but it has already established good international positioning in the field of multicomponent reactions and library design and production. Overall the quality of the work is very good. Both groups have a clear identity and a very good visibility but their partnership and synergy within the same Division could be improved. They are exploiting very efficiently fashionable waves (sustainability, MCRs, 'solar cells') but with a deeper rationale in their strategy, linked to the mission statements of the University and the Department. The collaboration with other teams in Amsterdam, elsewhere in the Netherlands and beyond is active, relevant and promising.

Productivity
The productivity is excellent with a stream of very good publications in high impact journals. The Division has a very good output of both international refereed academic publications and of PhD theses. Patenting could be pursued more vigorously.

Relevance
The work of this group is highly relevant, making an important contribution to the development of innovative methods and strategies in two different fields of organic synthesis and applicable both in academia and in industry. The methods that are developed to produce new compounds are original, elegant and efficient. The design of the target compounds and libraries would benefit from more strategic thinking in collaboration with biologists and molecular modelers.

Viability
This is a well set-up laboratory with an impressive national and international network and SBC appears destined to have an increasing impact on the field of organic chemistry, while OOC is perhaps currently too small to have critical mass. More involvement in rational design would reinforce SBC's position in chemical biology.

Conclusion

There is the basis of a strong group here with much potential to make an impact both in academic and industrial chemistry, but it could be larger to ensure critical mass and it needs to focus its chemical biology aspects more strategically and rationally.

Programme VU 5:	**Physical Chemistry**	
Programme director:	Prof. M.H.M. Janssen (Oct. 2005-2009) Imaging and Control of Photochemistry	
Research staff 2009:	2.4 fte	
Assessments:	Quality:	4
	Productivity:	4
	Relevance:	4
	Viability:	3

The group's mission is to advance the understanding and develop the control of nonadiabatic dynamics in photochemical reactions. The scientific objectives are threefold: (i) To integrate and utilize quantum-state selectors, ultrafast lasers, pulse shaping and position-sensitive electron- and ion imaging detectors in photochemistry. (ii) To study, manipulate, and control nonadiabatic effects in molecular photo-induced dynamics, with special interest in coherences from quantum interference. (iii) To foster the theoretical understanding and quantitative ab initio modeling of nonadiabatic photochemical dynamics by providing fully quantum resolved state-to-state three-dimensional angular-resolved scattering data.

Quality
The group is undertaking fundamental, innovative and original research into the nature of the reactions occurring within individual molecules that facilitates direct comparison with quantum mechanical theory. In addition, specially constructed equipment that allows the capture of femtosecond time resolution events occurring within molecules subjected to external control and manipulation, is being used to explore in real time nonadiabatic events with the objective of imaging and controlling chemical reactions. Publications have been in international journals of the very highest standing in physical chemistry and beyond. Although the citation rate during the review period is below expectations, it is important to note first, that Professor Janssen, who leads the group and is the only professor, was only appointed in 2006 and received full professorship in 2009, and second, that the group operates in a highly specialized area of physical chemistry. Evidence for the level of recognition of the high international standing of this currently nascent group is its membership in a consortium of leading European laser laboratories and in a leading EU Marie Curie-ITN network for imaging and control in chemistry.

Productivity
The external research income per fte is reasonably high, and balanced between national grants and EU contracts. Direct university funding has declined steadily during the review period. Viewed since 2006, the number of publications per fte in internationally refereed journals is high. The total number of Ph.D. students is small, but there are no dropouts, and the number per fte is high. The group has good resources in instrumentation and space. In addition, there is strong international collaboration and extensive networking with researchers in many centres, with some spending mini-sabbaticals with the physical chemistry group.

Relevance
As often with much fundamental investigation the current research is of primary relevance to academia in contributing to an understanding of the mechanisms of chemical reactions. The environment is important in training the next cadre of high quality research physical chemists to meet national needs, and several of the group members have gone into industry. Some of the specialty high-precision machined parts developed in the group have been sold to other research centres.

Viability

The group has been an important player in the previous Laser Centre at the university, now part of the new and large combined LaserLab Amsterdam, with UvA, and a player in LaserLab Europe. As a result, given its existing publication profile, it is anticipated that high quality research will continue. However, the group is very small, direct funding is declining, and yet the teaching of physical chemistry to both undergraduate and graduate students depends critically on this group. Although it receives support from its emeriti and has state-of-the-art equipment, it is questionable whether it can remain strong and viable at its present size. The department needs to give serious thought to its future.

Programme VU 6:	**Theoretical Chemistry**	
Programme director:	Prof. E.J. Baerends	Density Functional Theory Development
	Prof. F.M. Bickelhaupt	Theoretical Organic Chemistry and Biocatalysis
	Prof. L. Visscher	Quantum Chemistry and Multiscale Modeling
Research staff 2009:	12.2 fte	

Assessments:	Quality:	5
	Productivity:	5
	Relevance:	5
	Viability:	5

The research area of the Theoretical Chemistry group covers two coupled themes. In the first place, it aims at further development of molecular electronic structure theory, and of quantum chemical methods for the calculation of the electronic structure and the properties following from it. This research focuses on the physical models, numerical methods and efficient computer implementations. Density functional theory and methods are a central theme. Secondly, the Theoretical Chemistry group applies these methods to advance understanding of a variety of chemical phenomena. A focal point is the development of models and concepts for rational design in catalysis, (bio)chemistry and materials science.

Quality
This is a top leading research group both nationally and worldwide, with an outstanding reputation for its innovative, exceptionally high quality, and timely research. Its senior academic staff has received numerous coveted international awards and prizes, serve on the highest level national and global scientific committees, are on the editorial advisory boards of the top journals, and are frequently invited to address major scientific conferences. The quality of published output is exceptionally high. The group offers a coherent research programme addressing major scientific questions. It is well managed, and well endowed with financial and manpower resources.

Productivity
The group is dynamic and highly productive, with solid direct funding and an excellent level of research grants. It has a consistently high publication output per fte, and trains a reasonable number of Ph.D. students, although there have been some dropouts. It enjoys excellent supercomputing facilities, and it both collaborates with, and receives many guest scientists from, a large number of centres in Europe and throughout the world. It also collaborates strongly with, and is a resource for, the other groups within the department.

Relevance
The group is advancing fundamental knowledge in theoretical chemistry. The research of the group is very highly valued and represents valuable intellectual property, expressed through its spinoff company, with its density functional software sold to hundreds of research groups, and used by many more, in numerous areas of activity within industry, academia and government institutions worldwide. It provides excellent training in theoretical chemistry, and its Ph.D. and postdoctoral students are in heavy demand.

Viability
This is a large, very strong, young, and thriving group with rich resources and a clear future research strategy, both locally and internationally, which guarantees its future viability. It is a key player in local, national, and international centres and is a magnet for visiting scientists. Its leader is about to retire, but there is a sound succession plan, with a junior appointment in the same area

of research already in place. The only potential concern is the difficulty in attracting high quality graduate students into this demanding area of research.

9A. INSTITUTE LEVEL – Leiden University

University: Leiden University
Faculty: Faculty of Science
Institute: Leiden Institute of Chemistry (LIC)

1. Structure

The mission of the Leiden Institute of Chemistry is to perform fundamental chemical research and chemistry education at the highest level. The LIC aims to be an international and challenging environment where young talented researchers can develop their own research lines and where education and research are intimately intertwined. The research aims at contributing fundamental knowledge to important societal issues like sustainable energy and health and disease. The research programmes represent all the sub-disciplines of chemistry that are needed to facilitate the broad BSc programmes Life Science & Technology (LST) and Molecular Science & Technology (MST), both organized together with TU Delft).

The research is currently organised around two foci that allow for multidisciplinary approaches:

- Theory and Spectroscopy (aimed at sustainable energy)
- Chemical Biology (aimed at Health and Disease).

The Institute participates in two focal areas defined by the University: (1) 'Fundamentals of Science', and (2) 'Translational drug discovery and development'. Together with the Leiden University Medical Centre, the Institute has a leading role in the focal area 'Bioscience: the science base of health'.

Since November 2010, the LIC houses the Cell observatory, an initiative of the Faculty of Science. The Cell observatory brings together researchers from the institutes of Chemistry, Physics, Biology and Bio-Pharmaceutical Sciences. The goal of research at the Cell Observatory is to visualize and comprehend the dynamics of the living cell down to the molecular level.

2. Societal Relevance

The aim of the institute is to perform fundamental research, which means that the research results are usually far from direct valorisation. Still, the Institute has produced 48 patents in the period under review. Exploitation of this IP is performed in collaboration with LURIS (Leiden University Research and Innovation Services). To further develop the patent portfolio, a LURIS representative will be assigned full-time to the LIC management office.

In the opinion of the Institute, fundamental understanding is the only route towards real innovation. The results of fundamental research are of great value for society although they don't always lead to direct applications. The Institute expects that the Theory and Spectroscopy cluster will contribute to a fundamental approach of the problem of sustainable energy, whereas the Chemical Biology cluster will contribute to the development of new tools for medical research, new antibiotics and the identification of new drug targets.

3. Strategy for the future

In the period under review the LIC witnessed a reduction in tenured staff was accompanied by a substantial rejuvenation. Despite being smaller in number the staff have succeeded in enlarging the contribution of research grants and contract research to the budget considerably.

The additional funds of the Sectorplan will be invested in two full professors and two tenure track positions in the focus areas 'Chemical Biology' and 'Theory and Spectroscopy'.

The Institute notes that the growing awareness that the world's oil reserves are finite, has led to a political climate that will stimulate research in sustainable energy. The Institute expects that this will offer great opportunities for the focus area 'Theory and Spectroscopy' that aims at sustainable energy.

4. PhD Training

Within two months after appointment of a PhD-candidate, the promoter submits an Education & Supervision Plan (ESP) that describes the research and educational planning based on the specifics of the project and the background of the candidate. Advanced courses to deepen scientific knowledge are offered by the national research schools. The ESP also describes the teaching duties that are obligatory for every candidate. These teaching duties not only help the institute to run the BSc and MSc programs, but also offer the PhD students the valuable experience of direct contact with young students in an educational setting and the opportunity to develop their educational and communicational skills. All LIC PhD candidates are member of the Graduate school of Science organized by the Faculty. The graduate school of Science offers a program aimed at the development of more generic skills training, and personal effectiveness. This multi-year training program contains courses that are mandatory for all PhD candidates (Effective communication, Scientific integrity, Time management, Communication in Science), whereas other courses are optional such as e.g. Entrepreneurship.

The Committee notes the strong interaction of LIC with the TU Delft and the choice to focus on two broad research areas with high potential for the future. During the review period a number of changes have led to a higher focus on biorelated programs and a further broadening in the bio area with a potential risk of decreased attention to core chemistry aspects. An enhanced interaction between the programmes might lead to better coherence of the LIC. The successful implementation of the Cell observatory will further strengthen the interactions between physics, chemistry and biology.

9B. PROGRAMME LEVEL – Leiden University

Programme LEI 1:	**Bio-organic Synthesis (BIOSYN)**	
Programme directors:	Prof. H.S. Overkleeft	(2001-present)
	Prof. G.A. van der Marel	(2005-present)
	Prof. J.H. Boom	(2001-2004)
Research staff 2009:	19.8 fte	

Assessments:	Quality:	5
	Productivity:	4
	Relevance:	5
	Viability:	5

This is an excellent group, with broad expertise in carbohydrate, peptide, and nucleotide chemistry as well as in chemical biology. The group leader is young and dynamic and is supported by a team of outstanding co-workers, both at the professor and associate professor level as well as by a strong group of students.

Quality
The quality of this group is excellent. Its interests span a broad range of science from fundamental mechanistic studies in glycosylation methods to chemical biology and the design and preparation of new drug candidates. The group leader was designated the best organic chemist in the Netherlands under the age of 40 during the review period. The leader's talent is augmented by his excellent colleague Van der Marel and three more junior faculty members, with two Vidi grants between them in addition to the Vici grant of the group leader.

Productivity
The productivity of the group has been consistently very good over the entire review period both in terms of funding and publications. There are some high-profile hits amongst the large number of more routine synthesis and biological activity-test papers. However, there is comparatively little by way of obvious tokens of international recognition, such as presentations at major international meetings. This relative lack of recognition may be a function of the group's declared publication strategy: it may be that producing fewer, but more substantial publications in higher impact journals would have a positive impact all round on outside perception and will lead to more recognition.

Relevance
The synthesis of oligosaccharides and their bioconjugates remains an extremely challenging field and one of direct relevance to modern biology and medicine, since these molecules have powerful potential for probing cellular processes and possible therapeutically. The ability of this group to combine this synthetic expertise and that in the parallel fields of peptide and nucleotide chemistry with chemical biology increases this relevance further.

Viability
This group has excellent viability in terms of its research expertise, its ability to attract funding and top quality students, and a continued stream of quality publications. Its unusual blend of expertise in the bioorganic and chemical biology fields and the youth and ambition of its leader should ensure a bright future.

Conclusion

This is an all round excellent group whose only relatively minor weakness is its publication strategy whose pragmatic nature designed to help students in the short term is perhaps preventing the group from gaining the level of recognition to which it could aspire. A relatively minor adjustment here will be to the eventual benefit of all concerned.

Programme LEI 2:	**Biophysical Structural Chemistry (BSC)**	
Programme directors:	Prof. J.P. Abrahams (chair)	(2001-present)
	Dr. N.S. Pannu	(2002-present)
Research staff 2009:	9.28 fte	

Assessments:	Quality:	5
	Productivity:	4
	Relevance:	4
	Viability:	5

The research conducted by the group is on the frontier of modern structural biology. It is the aim to bring the field forward through development of experimental and computational technologies addressing challenging problems in structural biology. The group has been leading in establishing large shared national infrastructures; the most recent NeCEN (Netherlands Centre for Nanoscopy) at Leiden University giving the group unique opportunities to combine electron microscopy and X-ray crystallography to obtain 3D structural information on biological samples. Though the group contributes to structure determination of advanced biological projects it is not a typical "structural biology" group. The leaders have established an interdisciplinary environment, warmly appreciated by students, in which both software (EM / X-ray) and hardware (Crystallisation / EM) developments drive forward structure solution.

Quality
The Biophysical Structural Chemistry group is pioneering in the development of new methodologies for structural biology and is a top "methods" group worldwide both through the combination of different experimental techniques for structure determination of biological macromolecules and the development of novel software for both EM and X-ray analysis. The research is reflected in publications on extremely challenging experimental systems (the ribosome, F1-ATPase *etc*). The leadership in the field is also evident in the establishment and/or contributions to the cell observatory, the CytronI/II and the upcoming national centre for electron microscopy (NeCEN).

Productivity
Considering the quality of the research the productivity in terms of high profile research papers would be expected to be higher. The group attributes the move to the Cell Observatory to the apparent drop in productivity. Another measure of productivity is the groups contribution to the development of new computer algorithms found in widely distributed computer packages including those distributed by CCP4 (including REFMAC, CRANK, BP3, CRUNCH). The group has also produced EM software that give major improvements in signal/noise ratios as well as pioneering hardware developments in EM both at the sample preparation and analysis levels and the detector sensitivity.

Relevance
Three dimensional protein/macromolecular structural analysis is central both to academic science and to pharmaceutical and bio-science industries worldwide. Algorithms in widely distributed programme packages, to which this group contributes, thus aid society as a whole. . This multi-dimensional approach has established both facilities and software that can be widely accessed by the national and international communities.

Viability
The development of both new software and hardware for electron microscopy including electron diffraction as well as detector development, culminating in the establishment of a national centre

for electron microscopy (NeCEN) augurs extremely well for the future of this group. Recent developments in carbon nanotubes and the use of micro-crystals also look exciting areas for the future. Similarly, developments in X-ray structure determination protocols look strong, but this is an area where competing packages are always prevalent and the group must strive to keep above the competition in this area. The group is also encouraged to try and facilitate more local collaboration and synergy in the area of more routine structural analysis of proteins of interest to the diverse groups in Leiden. Grant funding for this group is exceptionally strong, reflecting the status of the Biophysical Structural Chemistry group.

Conclusion

The Biophysical Structural Chemistry group is tackling major challenges in structural (bio)chemistry and is at the vanguard of recent developments in both the hard and software for electron microscopy as well as single-crystal X-ray diffraction. The future looks extremely bright in terms of opportunities for excellent "local" science and for the establishment of world-leading international facilities. The Committee believes that the elements are in place for a successful future.

Programme LEI 3:	**Catalysis and Surface Chemistry (CASC)**	
Programme directors:	Prof. M.T.M. Koper (chair)	(2005-present)
	Dr. L.B.F. Juurlink	(2000-present)
	Prof. M. Bonn	(2000-2005)
	Prof. A.W. Kleyn	(2000-2005)
	Prof. B.E. Nieuwenhuys	(2000-2009)
Research staff 2009:	12.75 fte	

Assessments:	Quality:	4
	Productivity:	3
	Relevance:	4
	Viability:	4

This group is comprised of a group leader whose main focus is the study of electrocatalytic reactions, a tenured assistant professor working in the ultra high vacuum field, and their students. The common unifying theme of the group is the study of the reductive and oxidative cycles of carbon monoxide, oxygen, and nitrogen-containing compounds on surfaces. The group was strengthened by the addition of a Vidi supported assistant professor in 2007.

Quality
The quality of the group and its members is generally very good. It has a high degree of grant support, viewed as a percentage of the whole and recent publications in top ranked journals. The collaboration between the electrochemical and surface science parts of the group is starting to generate joint publications.

Productivity
The productivity of the group is good to very good overall, but there is considerable disparity between the two sections of the group with the electrochemical arm being by far the more productive. It is understood that Dr Juurlink has been carrying a high teaching load but is to be hoped that the collaboration will begin to bear fruit in terms of increased numbers of significant joint publications.

Relevance
The logical development of electrocatalytic methods based on a fuller appreciation of surface phenomena is relevant to fundamental science and potentially to society.

Viability
The group has very good potential. However, its long term viability will depend on the ability to profit from the potential synergy between the two existing branches. While there are indications that this is already taking place, further consolidation is needed.

Conclusion
The combination of surface science and electrochemistry is good and fundamentally logical. It is to be hoped that the two main partners will be able to reap maximum benefits from this overlap. Koper already has a very good visibility but if a true synergy is achieved with Juurlink, the standing of the group will potentially be increased greatly.

Programme LEI 4:	**Metals in Catalysis, Biomimetics and Inorganic Materials (MCBIM)**	
Programme directors:	Prof. E.E. Bouwman (chair)	(Nov. 2009-present)
	Prof. J. Reedijk	(2001-Oct. 2009)
	Dr. S. Bonnet (tenure track)	(Oct. 2009-present)
Research staff 2009:	7.83 fte	

Assessments:	Quality:	5
	Productivity:	5
	Relevance:	5
	Viability:	3

This group is the continuation of the earlier excellent and widely reputed one of Professor Reedijk. The post-Reedijk emphasis continues to be on co-ordination chemistry but with somewhat different goals in mind. Thus, the focus is now on biomimetic chemistry and catalysis including homogeneous catalysis and its application, inter alia, to the conversion of biomass. A young assistant tenure track professor has recently joined the groups with the help of a Veni project and is conducting research in the ambitious but highly competitive field of the induction of unidirectional motion of biomolecules on model membrane surfaces.

Quality
Reedijk's work, which is included in the review period, is clearly excellent. There was and continues to be high international recognition for this highly reputed scientist. It is too early to judge the quality of the independent research of Professor Bouwman and even earlier to judge that of her young collaborator Dr Bonnet. It is clear that Professor Bouwman provides very close and caring supervision of her graduate students. This is admirable but also carries a risk as detailed below.

Productivity
The productivity of the group over the past funding period is excellent, but again this assessment is based largely on the work of Reedijk. It would be both unrealistic and unfair to expect Professor Bouwman to attain such levels at an early stage of her career as group leader. Nevertheless, Professor Bouwman clearly attracts numbers of good students and it is to be hoped that as she grows into her new supervisory role that her ambitions and her productivity will grow accordingly.

Relevance
Catalytic conversion of biomass has obvious societal relevance as does the development of new routes for the production of bulk industrial chemicals such as isocyanates, eta-caprolactam, and phosgene; however, we note that in industry the latter is generally produced on site by catalysed chlorination of carbon monoxide, and this process will be hard to beat.

Viability
The viability of the group will depend on the ambitions and success of the new group leader. It is too early to judge this but it will be necessary for Professor Bouwman to grow into her new role and to employ her obvious ability to attract funding to acquire the postdoctoral collaborators necessary to help her supervise a larger group of graduate students. Small groups are vulnerable because the unforeseen loss of a critical member can rapidly translate into a loss of productivity and visibility. The group leader needs to adjust her modus operandi accordingly.

Conclusion

This is very much a group in transition. Previous quality, productivity and to some extent relevance are based on the outstanding contributions of Reedijk, but the future is in the hands of Bouwman who has been placed in what is perforce a difficult situation. The new group leader has the obvious ability to attract funding and students but probably needs to expand her ambitions to suit her new role.

Programme LEI 5: **Molecular Systems Biotechnology (MBT)**
Programme director: Prof. G. Ph. Van Wezel (2009-present)
Research staff 2009: 8.2 fte

Assessments:	Quality:	no scores
	Productivity:	no scores
	Relevance:	no scores
	Viability:	no scores

Notice: The Molecular Systems Biotechnology (MBT) expertise group was only started after the formal visitation period, in January 2009

The Molecular Systems Biotechnology group is a newly (2009) established small group, who work in the general area of Streptomyces biology. The group was previously part of the MOLGEN group; the creation of this new group was initiated by the VICI grant to Prof. van Wezel. The overall aim of the research of the group is to provide insight into the regulatory pathways of actinomycete bacteria. The present focus is on two complementary research programmes, one in the microbial development of S*treptomyces* with focus on cell division and programmed cell death and another in molecular biotechnology which focuses on the use of Streptomyces for the production of novel antibiotics. The group is engaged in collaborations with several other groups at Leiden Institute of Chemistry.

Quality
The research driven by Prof. van Wezel is highly visible in the *Streptomyces* field. Among the recent achievements in the programme are identification of the role of two *Streptomyces* proteins SsgA and SsgB proteins, linking them to establishment of the septum at cell division through direct (SsgB) and less direct (SsgA) interactions with FtsZ. The future will reveal the significance of these results in the general field of cell division. Collaborative work on the DasR regulator and its role, via *N*-acetylglucosamine, in linking nutrient stress to antibiotic production is highly regarded in the field. The programme on the development of novel antibiotics from *Streptomyces*, "awakening sleeping antibiotics" has the scope to be internationally competitive.

Productivity
Productivity, as far as can be judged from such a recent group formulation and bearing in mind past work within the MOLGEN programme, appears sound. The group will benefit from being embedded in the Cell Observatory, where it will bring expertise and equipment in fluorescence microscopy that complements the other imaging facilities in the Institute.

Relevance
The industrial uses of *Streptomyces* bacteria are considerable; from an expression host for the production of proteins through to the obvious role of this organism as an antibiotic factory. The group has industrial collaboration with the local site of a US/Danish enzyme producer (Genencor-Danisco) and is establishing programmes in antibiotic discovery. Both these aspects are of great societal relevance.
Viability
The viability of the group seems good. The future research portfolio seems strong and the activities of the group are well supported by mid- and long term funding. The antibiotic discovery programme is exciting, but antibiotic discovery is a competitive field with other well established major groups.
Considering the biological nature of the research programme the Committee felt that its position in the Leiden Institute of Chemistry appeared mainly justified by the antibiotics programme.

Conclusion

This is a newly established research grouping following the award of a VICI grant to Prof. van Wezel. The future looks strong but there are certainly challenges ahead as the group strives to compete in the antibiotic arena and to raise their game in the fundamental Streptomyces biology work.

Programme LEI 6:	**Molecular Genetics (MOLGEN)**	
Programme director:	Prof. J. Brouwer (chair)	(2001-present)
	Prof. M.H.M. Noteborn	(2008-present)
	Dr. R.T. Dame (tenure track)	(2009-present)
	Dr. R.C.L. Olsthoorn	(2007-present)
Research staff 2009:	15.92 fte	

Assessments:	Quality:	3
	Productivity:	3
	Relevance:	3
	Viability:	3

The current Molecular Genetics (MOLGEN) group is based around the research areas of the three most recent appointees Dr. Dame (in 2009), Prof. Noteborn (in 2008) and Dr. Olsthoorn (in 2007). The group, in its current incarnation, has evolved from the remains of terminated or merged programmes in DNA repair and Gene Expression. Prof. van Wezel was part of MOLGEN from 2007-2009, but has since moved to establish a separate group in Molecular Systems Biotechnology (LEI5), assessed separately. The research of the Molecular Genetics, which is strategically positioned in the general areas of DNA/RNA structure and cell death falls into the three subprograms:

- Chromatin organization and dynamics (led by Dr. Dame)
- Prediction, function and evolution of RNA structure (led by Dr. Olsthoorn)
- Tumor-selective activities of the chicken-anemia virus derived protein apoptin (led by Prof. Noteborn).

Quality
The assessment of the quality is primarily based on the material provided in the self evaluation report.
As such, quality of the research assessed is sound. The present state of the group reflects the measures that have been taken during the last couple of years to raise the quality of the research, e.g. merging of groups and termination of the internationally weaker programme in DNA repair. It is still too early to see the effects of the reorganization and the recent appointments on the quality of the research in the MOLGEN, but the Committee is expecting to see considerable advances during the next period.

Productivity
The many changes during the evolution of this group, coupled to the location of some of the students in the Leiden Medical Institute, make it difficult to assess the productivity of the group. Furthermore, the productivity analysis risks being strongly influenced by terminated research programmes with potentially fewer contributions from more recent staff, who now form the nucleus of the current activities. With these caveats, the productivity over the entire assessment period can be classified as good. The recent reorganization and the integration of two of the groups in the Cell Observatory are likely to catalyze an improvement of the productivity already in the medium term. A challenge of the group is how to nurture a more equilibrated enhanced productivity.

Relevance
The outreach activities, of Noteborn especially, are noted by the Committee who appreciate the enthusiasm and drive to work with the community in communicating the excitement of molecular genetics. These are extremely commendable activities especially at a time when funding levels are threatened and science is all too poorly understood by the general public and their

politicians. Work in the MOLGEN group is fundamental in nature, but translational applications in human health are certainly possible in the areas of viral RNA structure and programmed cell death but this will demand a far greater basic understanding than at present.

Viability

The newly established group in bacterial chromatin structure seems a viable area whose past productivity should continue to blossom. Work on RNA structure seems sound and may well find new life in studies of the influenza virus RNA packaging and its potential, when thoroughly understood, to act as a target for therapeutic agents although much work remains to be done before this is a reasonable proposition. Apoptin research remains a niche area with little external recognition and it will be interesting to see how this develops in the future in terms of international recognition and funding. There are good synergistic, links of this MOLGEN group with cell observatory which augers well for the future. The cell observatory interactions are justification for this grouping being placed in a Chemistry institute, but as with Molecular Systems Biotechnology, the marriage appears inappropriate in other ways.

Conclusion

The Molecular Genetics (MOLGEN) group is mainly focussed on the fundamental nature of DNA and RNA structure. Research is focussed around three comparatively recent appointments whilst the assessment is heavily biased by past research directions which are no longer considered viable.

It will be important for this current MOLGEN group to establish robust funding and internationally-significant publications for the University of Leiden, if it is to remain viable. It is hoped that the recent appointments provide the catalyst for the required improvements.

Programme LEI 7:	**Protein Chemistry**	
Programme directors:	Prof. M. Ubbink (chair)	(2001-present)
	Prof. G.W. Canters	(2001-2007)
	Dr. G. Siegal	(2001-present)
Research staff 2009:	13.74 fte	

Assessments:	Quality:	4
	Productivity:	4
	Relevance:	5
	Viability:	4

The Protein Chemistry group has evolved (starting in 2008) from the old grouping "Metalloproteins" which was successfully headed by Professor Gerard Canters. Since 2008 the Protein Chemistry group has been headed by Prof. Ubbink. The focus of the group was also changed from metal-protein interactions to investigations of protein dynamics and the interactions of proteins. NMR spectroscopic methods are the prime tool for these investigations but a variety of other biophysical techniques is also employed by the group. The focus of Prof. Ubbink's research is on protein complexes of redox proteins using paramagnetic effects. The studies of protein-small molecule interactions headed by Dr. Siegal represent another line of research in the PC group. This is an area important for drug developments, and a new ligand screening method and NMR hardware has been developed that has laid the foundation for a spin-off company.

Quality
The research of the PC group is of high originality in the employment and development of paramagnetic NMR techniques to study also large transient protein complexes. It is also innovative in the employment of different biophysical techniques to investigate the electrochemistry and redox chemistry of proteins. Protein-protein interactions studies, fragment based drug design, the analysis of transient complexes including those involved in electron transfer are all of a very high standard.
The group is clearly nationally leading in the research field using the application of NMR and other biophysical techniques to investigate proteins and protein interactions and possesses the potential to reach an internationally leading role in the field.

Productivity
The scientific output of the PC group was considered by the Committee be very good. It was noted that the part time appointment in the spin-off company has had a negative impact on the scientific productivity of Dr. Siegal in the evaluation period. With his return in a full time position this situation will hopefully be improved. The productivity of the PC group depends heavily on the availability of the research infrastructure at Leiden University in particular the NMR department. Considering the quality of the research the Committee would like to encourage a higher international profiling for some of the staff in this group and would advise more exposure at the relevant chemistry/biology meetings as well as at NMR methods meetings.

Relevance
The work of the Protein Chemistry group has considerable societal relevance. The use of NMR methods to study fragment binding to therapeutic targets is well established principle across the pharmaceutical industry. The TINS approach of Siegal has led to a successful spin-out company ZoBio which has synergistic and financially-important interactions with the University. The fundamental work on transient protein-protein interactions, protein-ligand interactions and on low occupancy transient-states, is at the forefront of a major emerging area in drug design and

medicine. There are clear applications in drug design across a range of targets as well having potential to probe the molecular bases for protein mis-folding diseases.

Viability

This group had to re-establish itself following the departure of Prof. Canters. The funding and a strategy for the future are in place and it will be important to re-establish Dr. Siegal at a higher academic profile upon his return from industry. The group is well integrated in the Institute and is part of the chemical biology theme in the Sector plan. One of the major needs of this group is the provision of high-field NMR in Leiden. This is essential both to allow the necessary scientific evolution of the work of this group and also to facilitate any new appointments in this area. Prof. Ubbink has developed a "road-map" for the development of NMR and other protein-interaction methods across the Netherlands and his drive in this initiative was appreciated by the Committee.

Conclusion

The Protein Chemistry group is a relatively new grouping that has evolved out of the previous metalloproteins group. The group has adapted well to the departure of Prof. Canters and has established its own niche studying the dynamics and interactions of proteins and their diverse complexes. The future looks bright, but the need for more access to high field NMR spectrometers is important for the evolution of the group.

Programme LEI 8:	**Soft Matter Chemistry (SMC)**	
Programme director:	Prof. J.G.E.M. Fraaije (chair)	(2001-2009)
	Dr. A. Kros	(2002-2009)
Research staff 2009:	6.3 fte	

Assessments:	Quality:	3
	Productivity:	3
	Relevance:	4
	Viability:	4

The Soft Matter Chemistry group centres around four researchers who have a common interest in lipid surfaces and biological membranes in the context of self-assembling systems. The vision of the group is to link the areas of physical and theoretical studies of soft matter systems to a more organic supra-molecular approach. Kros provides the organic and supra-molecular expertise whilst Fraaije and Sevnik provide theoretical models of membrane structure and dynamics and on block co-polymers, and Blokhuis focuses on mathematical analyses of membrane rigidity. The modelling component thus covers a wide-spectrum of modern techniques from field-based models through to a more atomistic approach.

Quality
The quality of work produced by the group covers a large spectrum which, on average, was assessed as "good" by the Committee. The recent work of Kros is clearly of very high quality; the other members of the group have a very low academic profile, with few publications, much of the effort apparently going into commercial software. The apparent lack of genuine collaboration or group coherence is disappointing for a group claiming a collaborative vision at its heart.

Productivity
Recent years have seen a surge in productivity for Kros, following a long lag period. Kros has a number of exciting high profile publications following the establishment of his "reduced-SNARE" method for fusing biological membranes. Academic productivity from other staff is much lower. Fraaije has established a company, CULGI, which develops and sells software for "multi-scale chemical modelling" for industry but this provides only indirect benefits to the academic SMC group, such as acting as an industrial partner for EU initiatives. The group would benefit from more exposure at international conferences, the current level of "invited lectures" being incompatible with the group's aspirations.

Relevance
The chemistry of membrane and gel systems is both an exciting area of fundamental science but also one with considerable application for drug delivery systems. There could be major developments for society as a whole, should this work evolve as hoped. Clearly the modelling work is of industrial interest, notably through the CULGI spin-out company, and through the network of industrial partners of the director.

Viability
The experimental work of Kros, notably with funding from the ERC, a VENI grant and as a partner in the SMARTMIX project, seems well set for the future. Indeed, currently the nine PhD students in the SMC group are all associated with Kros. The absence of bright young motivated students in the other areas must be considered a serious threat to the viability of the current SMC group. The future viability of the SMC group demands a far greater synergy between the

scientists than is currently evident and may also require a re-balancing of the synthetic and modelling components.

Conclusion

The SMC group has been built up over the years with a vision to take soft matter chemistry from mathematical modelling, through physical techniques to supra-molecular chemistry and vice-versa. A far greater synergy and coherence is essential for the long term viability of the group.

Programme LEI 9: **Solid State NMR/Biophysical Organic Chemistry (ssNMR/BPOC)**
Programme director: Prof. H. de Groot (2001-present)
Research staff 2009: 11.88 fte

Assessments:		
	Quality:	4
	Productivity:	4
	Relevance:	4
	Viability:	4

The group focuses on the development of methods for solid state NMR spectroscopy at high fields and the application of these tools to the solution of problems in structural biology and biophysical organic chemistry. Current work is directed at the study of proton coupled electron transfer in bacterial reaction centres, toward the preparation of artificial photosynthetic devices, understanding the electronic structure of photosynthetic reaction centres, in vivo magnetic resonance microimaging, the development of nanosecond 13C photo-CIDNP MAS NMR, and other problems including the study of charge transfer antenna by the incorporation of polarizability into the systems under study.

Quality
The group is comprised of a charismatic, ambitious leader assisted by three tenured staff with one Vidi and three Veni awards between them. This provides a dynamic and challenging environment for the 7-8 current graduate students and especially for the more ambitious among them. Funding is down from the peak in 2008 and the repeated claims of the group's field and world leading status have not yet borne fruit in terms of the award of major prizes other than the aforementioned Veni and Vidi awards.

Productivity
The productivity of the group is generally very good with a number of publications in excellent journals. It is somewhat puzzling that with the resources available to the group and the obvious ambition of the leader productivity has not been higher and recognition not more extensive.

Relevance
The development of artificial photosynthetic devices is potentially a very important goal for society, as is the development of the underlying understanding of the electronic structure of photosynthetic reaction centres and the workings of charge transfer antennae. Magnetic resonance microimaging could also be an area of broad relevance.

Viability
There is concern about the recent fall-off in funding and the low proportion of funding derived from research grants. This is however mitigated by the leadership in the recently awarded TBSC project on biosolar cells. The second concern arises from the project leader's own comments in the self-study document about the levels of ambition among the group's personnel and the inability of current staff to fill existing or projected gaps.

Conclusion
Overall, this is a potentially excellent group pursuing what are clearly ambitious goals with very good means to do so at their disposal. The group leader is rather outspoken in his comments, written and oral, and one cannot help but wonder if ultimately this pattern is detrimental to the group's productivity. With the lofty goals, the quality of the younger group members and the recently announced funding success one would hope to see increased productivity with retention of quality.

Programme LEI 10:	**Theoretical Chemistry**	
Programme director:	Prof. G.J. Kroes (chair)	(2001-2009)
	Prof. M.C. van Hemert	(2001-2005)
	Dr. J. Neugebauer (tenure track)	(2009- present)
Research staff 2009:	9.39 fte	

Assessments:	Quality:	4
	Productivity:	3
	Relevance:	4
	Viability:	5

Work in the theoretical chemistry group focuses on the areas of the dynamics of molecule-surface reactions, particularly the quantum dynamics of dihydrogen dissociation, and on the mechanism of photosynthesis with emphasis on the LH2 of purple bacteria. The aims are to achieve the ability to predict the outcome of surface-molecule reactions and to develop algorithms for the determination of mechanisms in functional photosynthetic devices.

Quality
A high quality young group leader, who has established a strong reputation, leads this programme. He has recently been joined by an excellent young tenure track associate professor who is supported by a VIDI grant that he obtained in 2009. The group leader has recent publications in very prominent journals, has been the vice-chair of a recent Gordon conference on surface Dynamics, and will be the chair of the same in 2011. Funding for the group has generally been very good, with a gradual but continuing increase in absolute levels over the review period. Currently, 72% of the group's fte's are supported by grant income.

Productivity
Productivity is good but has fallen off from a peak in 2005. This drop in productivity is in part due to the departure of one senior group member in 2005 and in part due to the group leader having been ill for a considerable time in 2006 and 2007. The group is aware of this problem and has taken steps to remedy it. The recent addition of an excellent tenure-track person should also contribute to increased productivity in the coming years.

Relevance
The study of surface phenomena is an important area as is the understanding of the mechanisms of photosynthesis. The development of new and improved computational methods, as well as their application, is of continued importance.

Viability
The young dynamic group leader and the recent addition of a highly competent tenure track person, combined with the good funding track record, strong research areas and increased focus on productivity, suggest excellent viability for this group in the coming years.

Conclusion
This is a generally very good group that has suffered in productivity owing to the departure of a group member and an illness. With the addition of an assistant professor and the return to productivity of the group leader the outlook and viability of this group are seen as excellent.

Appendix: Short profile of the committee members (in alphabetical order)

Bernd Bukau is Director of the Centre for Molecular Biology of Heidelberg University. His research group aims to understand the functional network of chaperones and proteases in the cytosol, using bacteria, yeast and mammalian cells as model systems, and combining genetics and cell biology with biochemistry and biophysics as experimental approaches.

Robert Cava is Professor of Chemistry and Materials at Princeton University and Chair of the Department of Chemistry. His research group studies the chemistry of materials, emphasizing the relationships between chemistry, crystal structure and electronic and magnetic properties of non-molecular solids.

Chris Chidsey is Associate Professor of Chemistry at Stanford University. The Chidsey group research interest is to functionalize electrodes for molecular electronics and electrocatalysis. They synthesize molecular and nanoscopic systems, build the analytical tools and develop the theoretical understanding to study electron transfer between electrodes and among redox species through insulating molecular bridges.

Brad Chmelka is Professor of Chemical Engineering at the University of California Santa Barbara. His research includes the correlation of macroscopic material properties and function with molecular structure and dynamics, particularly in heterogeneous macromolecular solids using techniques of NMR spectroscopy.

David Crich is Director of the Institut de Chimie des Substance Naturelles (ICSN), Gif-sur-Yvette, France. His research expertise is on organic chemistry, synthetic methodology and total synthesis.

Edward Cussler is Professor of Chemical Engineering at the University of Minnesota. His research expertise is on chemical separation processes, thin films, membranes and module design.

Gideon Davies is Professor of Chemistry at the University of York. His expertise is in structural enzymology and carbohydrate chemistry. Research in the Davies group is focused on the structural enzymology and biological chemistry of the enzymes that are involved in the synthesis, modification and breakdown of carbohydrates.

Gunnar von Heijne is Professor in Theoretical Chemistry at Stockholm University and Head of the Center for Biomembrane Research. His research covers biochemistry and molecular biology, especially membrane proteins. He has explored and developed new theoretical methods to predict membrane protein topology and 3D structure in both prokaryotic and eukaryotic models.

Marcel Hibert is Professor in the Faculty of Pharmaceutical Sciences at the University of Strasbourg, and Director of the Laboratoire d'Innovation Thérapeutique. His research focus is on drug design and developing novel strategies and technical platforms to rationalize and accelerate the discovery of ligands acting on genomic targets.

Héribert Hirt is Professor of Molecular Biology at the University of Vienna and Director of the URGV Plant Genomics Research in Paris. His research interests include signal transduction of abiotic and biotic stress.

Kurt Kremer is Director of the Max-Planck Institut für Polymerforschung in Mainz. His research employs various computer simulation techniques to study problems in soft matter

physics.

Sine Larsen is Professor of Structural Chemistry at the University of Copenhagen and Director of the MAX IV laboratory in Lund, the National Swedish Synchrotron Laboratory. From 2003 to 2009 she was the Director of Research at the European Synchrotron Radiation Facility in Grenoble. Crystallographic methods form the basis for most of her research in structural chemistry and structural biology. Presently she is the President of the International Union of Crystallography.

Malcolm Levitt is Professor of Chemistry at the University of Southampton. His research is on the methodology and applications of nuclear magnetic resonance (NMR) in the solid state, especially biological materials.

Josef Michl is Professor of Chemistry at the University of Colorado. His research group works in physical organic chemistry. They synthesize organic and organometallic compounds and investigate their properties by physical, mechanistic and computational methods. This ranges from photochemical reactions to nanotechnology. He has co-authored five books on photochemistry and polarization spectroscopy, and many scientific papers in the areas of organic, inorganic, theoretical, and physical chemistry.

Ka Ming Ng is Chair Professor of the Department of Chemical and Biomolecular Engineering at the Hong Kong University of Science and Technology (HKUST). He also serves as the CEO of the Nano and Advanced Materials Institute. His research interests are in product conceptualization, process design and business development involving water, biochemicals, natural herbs, polymers, pharmaceuticals, semiconductor materials, and nanomaterials.

Janusz Pawliszyn is Professor of Analytical Chemistry at the University of Waterloo. His research focus is on the development and application of state-of-the-art, integrated and automated analytical methods and instrumentation, for on-site analysis and monitoring.

Malcolm Rowland is Professor Emeritus and former Dean of the School of Pharmacy and Pharmaceutical Sciences, and former director of the Centre for Applied Pharmacokinetic Research, at the University of Manchester. His main research interest is physiologically based pharmacokinetics and its application to drug discovery and development.

Jeremy Sanders is Professor of Chemistry at the University of Cambridge and Head of the School of Physical Sciences. In 2006-2010 he was Deputy Vice-Chancellor of the University of Cambridge. In 2004-2008 he was Chair of the Chemistry panel of the Research Assessment Exercise (RAE). His research group is interested in molecular recognition, aiming to uncover and exploit the rules governing non-covalent interactions.

Frans De Schryver, chairman of the Committee, is emeritus professor and guest professor at the Catholic University of Leuven. His research has focused on the fundamental aspects of photochemistry and photophysics and their use in the study of the physicochemical properties of complex systems. During the last 10 years he contributed primarily to the emerging field of time- and space-resolved (photo)chemistry, scanning probe microscopy, optical microscopy, single-molecule spectroscopy and nanoscience.

Peter Seeberger is Professor at the Free University of Berlin and Director of the Max Planck Institute of Colloids and Interfaces. From June 2003 until January 2009 he held the position of Professor for Organic Chemistry at the Swiss Federal Institute of Technology (ETH) in Zurich.

Appendix: Explanation of the SEP criteria and scores

The four main criteria for assessment are: Quality, Productivity, Relevance, and Vitality & feasibility. The assessment at the institute level primarily focuses on strategy and organisation, whereas the assessment at the level of the research group or programme primarily focuses on performance and activities of researchers and the results of their work (output and outcome).

Quality	The level or degree of excellence of the research, compared to accepted (international) standards in that field. The scope of the term 'research' is not limited to the research results. Research management, research policy, research facilities, PhD training and the societal relevance of research are considered integral parts of the quality of work in an institute and its programmes.
Productivity	The relationship between input and output, judged in relation to the mission and resources of the institute.
Relevance	Social, economic and cultural relevance. Aspects to be considered are: ▪ *Social quality*: efforts of the institute or group to interact in a productive way with stakeholders in society ▪ *Social impact*: how research affects specific stakeholders or procedures in society ▪ *Valorisation*: activities aimed at making research results available and suitable for application in product, processes and services. Remarks can also be made about the relevance for the academic community, but the assessment should be on societal relevance.
Vitality & feasibility	The ability to react adequately to important changes in the environment. Also vision for the future.

The scores on a five-point scale are:

5 Excellent	Research is world leading. Researchers are working at the forefront of their field internationally and their research has an important and substantial impact in the field.
4 Very Good	Research is considered nationally leading. Research is internationally competitive and makes a significant contribution to the field.
3 Good	Research is considered internationally visible. Work is competitive at the national level and makes a valuable contribution in the international field.
2 Satisfactory	Research is nationally visible. Work adds to our understanding and is solid, but not exciting.
1 Unsatisfactory	Work is neither solid nor exciting, flawed in the scientific and/or technical approach, repetitions of other work, etc.