Research Assessment 2016

Institute for Molecules and Materials

Radboud University
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1 Introduction

1.1 The Netherlands System of Quality Assessment of Research

All publicly funded research in the Netherlands is assessed regularly in accordance with the Standard Evaluation Protocol (SEP) published under the authority of the Association of Universities in the Netherlands (VSNU), the Netherlands Organisation for Scientific Research (NWO), and the Royal Netherlands Academy of Arts and Sciences (KNAW).

The primary aim of assessments under Standard Evaluation Protocol 2015-2021 is to reveal and confirm the quality and the relevance of the research to society and to improve these where necessary. This includes:

- Improvement of research quality, including societal relevance of research, research policy, research management, education and training of doctoral candidates, academic integrity and the facilities.
- Accountability to the board of the research organization, and towards funding agencies, government and society at large.

The present document is the report of an external committee of peers that evaluated the research quality of the Institute for Molecules and Materials of the Radboud University during a visit in November 2015.

1.2 The Members of the Evaluation Committee

The Review Committee consisted of:

- Prof. dr. em. J. Friso van der Veen (Chair), Paul Scherrer Institute, Villigen, Switzerland.
- Prof. dr. Alec Wodtke, Max Planck Institute for Biophysical Chemistry, Göttingen, Germany.
- Prof. dr. Viola Vogel, ETH Zürich, Zürich, Switzerland.
- Prof. dr. Stuart Parkin, Max Planck Institute for Microstructure Physics, Halle, Germany.
- Prof. Lucia Sorba, Director NEST, Instituto Nanoscienze-CNR, Pisa, Italy.
- Prof. dr. Walter Thiel, Max-Planck-Institut für Kohlenforschung, Mülheim, Germany.
- Dr. Rinus Broxterman, DSM, Geleen, Netherlands.

Dr. Hanneke (J.T.A.) Meij, Nijmegen, served as secretary of the Review Committee. Short curricula vitae of the Committee members are given in Appendix 1.
Impartiality
All of the Committee members signed a statement of impartiality declaring that they would judge without bias, personal preference or personal interest, and that their judgement is made without undue influence from persons or parties committed to the institute or programmes under review, or from other stakeholders.

1.3 Scope of the Assessment
The assessment was commissioned by the Executive Board of Radboud University. It covers research conducted by the Institute for Molecules and Materials (IMM).

The Institute for Molecules and Materials was formed in 2005 as one of the research institutes of the Faculty of Science at Radboud University. The first and most recent research assessment of IMM was carried out in 2008. The current Committee was charged with retrospectively assessing the quality of the research at IMM over the period of 2009-2014. In addition, it was asked to prospectively assess the strategic targets of IMM and the extent to which it is equipped to achieve them in the future. As the research programmes at IMM was redefined into four themes (see below) in 2012, this report is the first assessment of IMM in its new organisational structure.

Levels of assessment
The assessment was done at two organisational levels: the institute as a whole and the four research programmes or “themes”: i.e.,
Theme 1: Structure and Dynamics of Molecules
Theme 2: Molecular Life-like Systems
Theme 3: Quantum Matter
Theme 4: Materials Design
The Committee also provided recommendations for improvement at both the institute and theme level.

Assessment criteria
In accordance with Standard Evaluation Protocol 2015-2021, the Committee judged the performance of the institute and its research themes on the three criteria detailed below (paragraph 1.6), taking into account current international trends and developments in science and society.
1.4 Data provided to the Committee

A month before the site visit, the Committee members received a Self-evaluation Report from IMM. The first chapter covers the institute as a whole. It describes its mission, organisation and strategy; internal and external collaborations; scientific and societal developments impacting research; scientific staff and other personnel; resources; funding and facilities; provides performance indicators, research output, societal output; a SWOT analysis matrix, benchmarking, details on PhD student guidance and performance; policies regarding research integrity and strategy for the future.

The second chapter consists of detailed information about the four research themes. Each theme is described in terms of research area, mission, organisation and strategy; developments impacting the research; scientific staff and other personnel; resources; funding and facilities; performance indicators, research output and societal output; a SWOT matrix and strategy. Throughout the first two chapters, selected topics and/or publications are presented to illustrate the diversity and relevance of the institute’s output.

The Committee members also received a copy of the SEP 2015-2021 and Terms of Reference for the assessment. Copies of IMM publications, PhD theses and other documents, such as annual reports, were available to the Committee in the interview room. The documentation included all the information required by the SEP 2015-2021.

1.5 Procedures followed by the Committee

Ahead of the site visit, the Chair assigned one Committee member as primary expert on each of the four research themes and on the subjects of Theory and Industry (Valorization). Another member was designated as secondary expert. The Chair also asked the Committee members to read the Self-evaluation Report with their assignment in mind, and to send him their preliminary judgements on their primary research theme only, prior to the site visit. This distribution of work was meant mainly to ease the load before and during the visit, and to keep the discussions during and after the interviews, on target.

The Committee first met on the eve of the site visit, following a welcome by the President of the Radboud University (Prof. dr. G.J.M. Meijer), the Dean of the Faculty of Science and a delegation from IMM. In the closed preparatory meeting the Committee composed a list of interview questions and took further decisions based on the preliminary assessments and the IMM Self-evaluation report.
Specifically, it was agreed that each Committee member take the lead on their one assigned subject not only during interview and discussion, but also in writing the report. The Committee member assigned as secondary expert would add comments and edits. Thereby, every research Theme was assessed by two Committee members, both experts on the particular theme, and separately on Theory and on Valorization.

The actual site visit (for the full programme see Appendix 2) took off with a presentation on IMM as an institute by its Director, Prof. dr. Elias Vlieg, supported among others by the IMM Managing Director, dr. Freya Senf-Huijgen. For each of the four research themes, the Committee met with representative group leaders, one presenting a slide show and others supporting him/her during the interview. Printed as well as digital copies of each slide presentation were available on-site. The Committee also interviewed the Dean of the Faculty of Science, Prof. dr. C.C.A.M. Gielen, a delegation of PhD students and some of the Tenure-Track faculty members. Furthermore, the Committee members toured the labs and large facilities.

Since ample time had been planned between interviews for the Committee to discuss its findings and make notes, the final closed meeting proceeded efficiently. The Committee was unanimous in its comments and scores. Finally, the Chair presented the main conclusions to the IMM staff; the President of Radboud University (Prof. dr. G.J.M. Meijer) attended this meeting. Most reports were completed soon after the interviews, some took longer.

1.6 Criteria and Assessment Scale

In accordance with Standard Evaluation Protocol 2015-2021, performance was judged on the three SEP assessment criteria:

A. Research quality

The Committee assessed the quality and reputation of the research and the contribution that research makes to the body of scientific knowledge. The committee also assessed the impact of the research results (scientific publications, instruments and infrastructure developed by the unit, and other contributions to science).
B. Relevance to society
The Committee assessed the quality, impact and relevance of contributions targeting specific public or private societal actors by advisory reports for policy, by contributions to public debates, and so on. The Committee also assessed contributions to areas that the research unit itself has designated as targets.

C. Viability
The Committee assessed the strategy which the research institute intends to pursue regarding research performance and societal relevance in the years ahead and the extent to which the institute is capable of meeting its targets. It also weighed the governance and leadership skills of the research unit’s management in its assessment.

The qualitative assessments are supplemented by assigning discrete categories (1-4): Excellent (1); Very good (2); Good (3); Unsatisfactory (4). The meaning of the categories in this four-point scale used in the assessment is described in the Standard Evaluation Protocol (see Appendix 4).
2 Assessment of Institute for Molecules and Materials

Institute for Molecules and Materials (IMM)

Director of the institute: Prof. dr. Elias Vlieg
Academic staff in 2014: 185.8 fte
Assessment:
- Research Quality : 1
- Societal Relevance : 1-2
- Viability : 2

2.1 Mission, strategy, targets and research activities

The Institute for Molecules and Materials is an interdisciplinary research institute in chemistry and physics at the Radboud University. Its mission is to fundamentally understand, design and control the functioning of molecules and materials. The institute is a centre of excellence that trains the next generation of leaders in science and entrepreneurship.

The IMM distinguishes itself from similar institutes by the intense collaborations and interactions between chemists and physicists and/or experimentalists and theorists and the very strong infrastructure that includes large user facilities such as the High Field Magnet Laboratory (HFML) and the Free Electron Laser facility FELIX.

2.2 Research Quality

The IMM was introduced to the committee by its director Elias Vlieg in an inspiring opening presentation. The committee members were all impressed with what they heard during this presentation and later during their two-day visit. The committee also greatly enjoyed the presentations by the leaders of the four research themes which make up IMM, as well as the discussions with academic staff members and PhD students. The visit was well-organized, and the self-evaluation report was concise and informative. The committee thanks the support staff for their hospitality and efficiency, making it possible to have the full research program of IMM presented and evaluated during a site visit of only two days.

The committee commends IMM for being very successful in bringing together scientists with different backgrounds around a common research goal: “to fundamentally understand, design and control the functioning of molecules and materials”. We see a great collaborative spirit among the staff members and an inspiring environment for PhD students. The collaborative spirit is in our view the most important asset of IMM. A second major asset is the availability of an outstanding research infrastructure with unique facilities such as HFML and FELIX. Both
assets result in research programs within the four main themes of IMM that are in the categories “very good” or “excellent”/”world-leading”.

### 2.2.1 Academic reputation

The staff members of IMM have been very successful in the acquisition of individual research grants both at the European and the national level. We mention here the Spinoza awards and ERC advanced research grants for Rasing and Katsnelson and the ERC advanced research grants for Huck and Nolte. Noteworthy is also the Gravitation program “Functional molecular systems”, in which Van Hest and IMM colleagues participate within a consortium of groups from Nijmegen, Groningen and Eindhoven. IMM can also boast an increasing number of VENI, VIDI and VICI grants as well as ERC starting grants. The number of refereed publications and citations has also risen during the past years. The committee congratulates IMM with its success and high research standard.

### 2.2.2 Research infrastructure and facilities

The FEL facilities and HFML are unique research infrastructures to be proud of, and their operation needs adequate baseline funding. We learnt that HFML now runs for ca 2200 magnet hours per year, which is a significant increase relative to those in 2007, the year of the previous review. The goal is to increase this number to ca 3000 hrs per year. Technically, this is possible but at present there is no funding for the needed extra personnel. The FELIX lasers provided 3200 beam hours to users in 2015, and the aim is to maintain or even increase this number. Over 3000 hours of operation a year at these facilities is in line with operation conditions at user facilities elsewhere.

The strategy of HFML was well presented and clear. In 2013 Hussey succeeded Maan as director of HFML. A strong asset is the combination of the high fields with FELIX radiation. A 45 T hybrid magnet is under development, in collaboration with MagLab in Tallahassee, USA.

The committee would like to have heard more about the strategy for the FEL facilities. There was neither a presentation on the source and the machine properties, nor on their optimization for specific spectroscopy experiments. Ambitious plans should be formulated for further development of the sources and the beamlines during the coming 6 years, in order to create optimal conditions for ambitious science projects of both IMM groups and external users. Of course, the relocation of FELIX from Rijnhuizen to Nijmegen took a lot of effort and resources, but now the next steps have to be taken in order to keep the FELs at the forefront of science. We would recommend all theme leaders of IMM to further brainstorm on how to make the best possible use of these unique facilities. The vacancy left behind after the
departure of Van der Zande as leader of the FEL-facilities must be filled soon so as to ensure continuity.

The committee feels that the NMR field is losing some momentum. We recommend integrating NMR better with other strengths with respect to instrumentation.

2.2.3 Organization

The organization of IMM seems well optimized to achieve the stated goals. A flaw is that not all Themes are represented in the Board. This should be repaired.

The research activities facilities FELIX and HFML are strongly embedded (though not exclusively) in the themes SDM and Quantum Matter, respectively. One may thus expect that technical developments at the facilities are science-driven, as they should be. On the other hand, one may consider adapting the organizational structure such that the visibility of the facilities to stakeholders (FOM, NWO, EU) is enhanced. HFML is led by Hussey; the FEL-facilities need a new strong leader. It was not clear to the committee who formally represents the facilities in negotiations with stakeholders. Having committed spokespersons for those facilities with well-defined competences is important, because long-term funding prospects for large facilities are chronically insecure in a university environment not having the formal status of a ‘national laboratory’.

2.2.4 Resources

Over the past 6 years, the dependency of IMM on external funding has increased to 70-80% at present (mainly from NWO, FOM, EU). The IMM presently enjoys having a strong commitment from the University. Long-term funding of both HFML and FEL-facilities should ideally be shared between FOM/NWO and the University in proportions to be mutually agreed. It is the understanding of the committee that FOM pays for FELIX an annually decreasing contribution till 2021. Clearly, a long-term commitment for institutional funding of the expensive infrastructures should be sought in discussions at the highest level with NWO and the Dutch government. The impending fusion of FOM and NWO probably is a unique opportunity to get such a commitment. In these discussions, the interdisciplinary character of the research at the facilities is a unique major asset.

The committee heard about the Sector Plans in physics and chemistry and the Top Sectors. National grant application subjects now basically have to fit within the Top Sector plan, and it was unclear to the committee whether IMM has developed a specific strategy on this matter or whether this is left to the individual research groups. The same applies to the EU program
Horizon 2020, in which the utilization potential is essential, more so than the science. In the past, IMM has had great success with getting its basic science funded, but for the next 6 years it needs to develop a strategy on how to gradually shift research interests to subjects of higher direct utilization potential and on how to better valorize science results. In part, this is already happening within IMM, but not within all themes and not yet to the extent needed to fully tap into the resources made available by the funding agencies in these changing times.

2.3 Societal relevance

The prime mission of IMM is to perform fundamental, curiosity-driven research. Yet, a number of groups within IMM, notably the groups of Rutjes, Van Hest, Buydens and Huck within the theme "Molecular Life-Like Systems", have been very successful in the commercialization of their research, through the creation of spin-off companies or through participation in a public-private partnership (PPP). An excellent example is COAST (founding board member Buydens), with participation of more than 40 companies. An important initiative of both IMM and the academic hospital is the Radboud Nanomedicine Alliance, which focuses on regenerative medicine and targeted drug delivery. This initiative is an example of forward programming on societal impact. There are several other PPPs in which IMM participates at the national or regional level. There seem to be concrete plans to valorize the work in the Life Science Trace Gas Facility led by Harren. The ultrasensitive methodology can be leveraged in, e.g., medical diagnostics applications (biomarkers) and gas-surface diagnostics. We think this is important and worthwhile. The activity in high efficiency III-V solar cells has also been very successful in commercialization with the creation of four spin-off companies.

IMM has clearly identified that the funding landscape will irreversibly change. Valorization of the results of IMM was, and is, identified as a strategy to mitigate this change, and opens new avenues for funding. We encourage IMM to define more focal areas for possible PPPs, spin-offs and other valorization activities. At present, the strategy works out quite differently within the four themes. Within theme 1 there seem to be significant valorization options, the Trace Gas Facility being an example. It is wise to start creating a business plan for activities within theme 1 during the next 6 years. Within theme 2 the mind-set for valorization dates back to ‘pre-IIMM’ times, and valorization seems almost part of the everyday work. This creates significant societal impact, including spin-offs. Within theme 3, it is probably more difficult to valorize, but the potential for valorization is of a game-changing nature. There is significant valorization within theme 4, with patents, public-private projects and spin-offs.

We see a need for more guidance from the University Board and IMM management on how to implement specific elements of valorization. For example, one needs more clarity regarding a
possible percentage of ownership of spin-offs by staff members and the amount of time that can be spent with these start-ups. One also wants to understand why the University currently does not want to take ownership shares in companies. We advise IMM and the University to think about creating ways to earn back more in a direct manner on valorization. Owning a small part of the start-ups is one of the most direct earn-back mechanisms.

As regards human resources, it is important that mechanisms are in place to keep the staff fully motivated. IMM has been doing very well in this respect, and its scientists are generally strongly self-motivated, as one may expect in centres of excellence. We were informed about the tenure-track system at IMM and we learnt that tenure track will not ultimately lead to the rank of full professor, not even in the case of very good performance. We understand the underlying reasoning; IMM does not want too many independent professorships, this not being in the spirit of collaboration within IMM. However, we believe it would be wise to have some flexibility in the system, so that exceptional talents can be kept. Concerning gender balance and hiring of female staff, IMM policy seems in line with good practices elsewhere: advertising, active scouting, strategic funds to keep female candidates, maternity leave, day-care centre, and mentoring.

2.4 Viability

Given the successes of IMM during the past 6 years, we recommend continuing with the same organizational structure for the institute and with the same set of research themes. However, for theme 4, Materials Design, one would need to rethink the strategy. As stated before, staff working in all themes, particularly theme 2, should brainstorm on how make best possible use of the large facilities on campus. One also needs to make an inventory of research opportunities within the Dutch Top Sectors.

2.5 PhD programmes, training and supervision

During the two-day visit the committee had the opportunity to have lunch with 6 PhD students. Overall, the students were very happy with their working conditions and with the guidance provided by their supervisors. They were also satisfied with the freedom they were given in their research.

Responsibilities regarding supervision seem properly defined. In a number of cases, daily supervision is not by the professor but by an intermediate person from the staff, e.g. an assistant or associate professor. This seems fine, as long as such arrangements are mutually agreed upon, effective and periodically reviewed. The committee learnt that there is a formal Training and Guidance Plan in place. Regarding the PhD trajectory, there is a “go-no-go”
decision after the first year of employment. The students are aware of this, but only in rare cases it comes to a no-go. For a thesis, it is generally required to have 3 publishable chapters. One should finish the thesis work within 4 years; in fact, one gets a financial bonus if this happens. It is laudable that specific steps have been taken to minimize delays. In the past years progress has been made with reducing the average duration of a PhD-period, which presently is 4.5 years.

Several training courses are offered to the students. We heard that a course on time management will be mandatory. We were surprised to hear that IMM offers PhD-students no course on entrepreneurship. The students told us, they would enjoy such a course.

Overall, the committee finds that the organization of the PhD programmes, the training and the supervision are of high quality. The PhD-theses are of a high international standard. Generally, persons with a PhD-degree in physics or chemistry from The Netherlands are much-wanted as employees both nationally and abroad.

2.6 Policy on academic integrity

From the documents provided the committee took note that a code of conduct is in place. We agree that a course on Scientific Integrity should be part of the educational programme for all PhD students.
3 Recommendations regarding Institute for Molecules and Materials

3.1 The quality of the research institute as a whole

The Committee recommends the following:

- Strengthening of the organizational structure as regards facility management, in particular the management of the FEL facilities. Securement of long-term funding prospects for the large facilities by negotiation with agencies, using the impending fusion of FOM and NWO as a window of opportunity.

- More ambition in matching FEL machine properties to future science needs. Broader use of FELs across themes. Rethink future of solid-state research.

- Keep momentum in NMR.

- Enhance gender balance in the faculty.

- Developing a strategy on how to gradually shift research interests to subjects of higher direct utilization potential and on how to better valorize science results.

Regardless of the required move towards increased valorization, the Committee emphasizes the need for basic curiosity-driven research such as has been performed successfully at IMM in the past, because that kind of research provides fundamental new insights and breakthrough discoveries, which best serve society in the long run.

3.2 The institute's PhD programmes

The Committee recommends the following:

- Further reduction of the average duration of a PhD-trajectory.

- Course in entrepreneurship.

3.3 The unit's research integrity

The Committee recommends the following:

- Adhere to Code of Conduct.

- Continue with making the students aware of the subject. Use of software for identifying possible plagiarism.
4 Assessments per programme

4.1 Theme: Structure & Dynamics of Molecules

<table>
<thead>
<tr>
<th>Leader:</th>
<th>N/A</th>
</tr>
</thead>
<tbody>
<tr>
<td>Academic staff in 2014:</td>
<td>39.3 fte</td>
</tr>
<tr>
<td>Assessment:</td>
<td></td>
</tr>
<tr>
<td>Research Quality</td>
<td>1</td>
</tr>
<tr>
<td>Societal Relevance</td>
<td>2</td>
</tr>
<tr>
<td>Viability</td>
<td>2</td>
</tr>
</tbody>
</table>

Research Quality

Nijmegen’s early stage profile was strongly influenced by excellence in molecular spectroscopy. It is, therefore, no surprise that the “Thematic Group: Structure and Dynamics of Molecules” (SDM) has been very successful and visible within the IMM (and during the years before IMM was established). Development and demonstration of spectroscopic methods like Velocity Map Imaging and Cavity Ring Down Spectroscopy have become known worldwide and are now used ubiquitously in physics and chemistry. The success of these methods as well as other experimental work supply a strong international profile for Nijmegen’s gas-phase molecular physics and physical chemistry faculty. Theoretical activities in quantum dynamics have complemented the experimental work in a way that makes both experiment and theory more valuable. The theoretical research in this area is of high quality and clearly goes beyond the mainstream of computational chemistry. The Trace Gas Institute also provides a strong profile for the whole campus and can be regarded as one of its flagships. The external funding of the SDM group has grown strongly (by more than a factor of 2 since the last review!). Scientific output has grown proportionately. Publications appear in the best journals.

The Committee considers the research quality of Theme 1 world leading and excellent and, therefore, of category 1.

Societal relevance

Gas-phase molecular physics and physical chemistry belong primarily to the realm of basic research aiming at the fundamental understanding of Nature. It is thus noteworthy and impressive that the Trace Gas Facility has been able to pioneer societally relevant research in this field, with significant medical applications such as breath analysis on the horizon. Applications of high resolution and ultrasensitive spectroscopy have been expertly developed under the leadership of Harren.
The move of FELIX to Nijmegen has opened new options for societally relevant research, for example by employing mass spectrometric methods in combination with FELIX. Even in the early days of FELIX operation in Nijmegen, contacts to the medical school have been made and new research directions have been initiated. Another exciting new research direction is surface dynamics at ices (funded through a prestigious CW-TOP grant). Generally, the field of surface chemistry and dynamics offers great opportunities for work of societal relevance.

The Committee considers the societal relevance of Theme 1 very good and, therefore, of category 2.

Viability

Excellent young hires within SDM and IMM are signs of a promising future. We are particularly pleased to see that the field of “Cold Molecules”, which was “made in the Netherlands”, has returned to Nijmegen in an outstanding style (van de Meerakker). The new research area of surface dynamics at ices is strengthened by the recent hire of an assistant professor in theoretical chemistry (Cuppen) that is also active in a different thematic group (“Materials Design”), which exemplifies the advantages of the collaborative environment that the IMM has successfully created.

The FELIX has moved and is now open for business in Nijmegen. We consider the SDM group to be the natural intellectual owner of this new facility, which is capable of providing essential contributions towards making FELIX a high-profile success on an international scale. Strong theoretical support and the hiring of excellent faculty will be needed to achieve this goal.

We believe that the advent of FELIX provides an opportunity for the successful development and evolution of the SDM thematic group over the long run, with increasing focus on complex systems of relevance to physics and chemistry. While not all SDM scientists should be expected to be “FELIX scientists”, all of the groups within the SDM theme can and should contribute to the success of FELIX in Nijmegen. Future hires should be used to strengthen the position of FELIX and to exploit its potential. We are concerned that SDM professorships are being phased out (Parker and Harren) at the time when FELIX is coming on line, especially when considering the intrinsic scientific links between SDM and FELIX. This leads us to recommend that the Parker and Harren positions be retained for SDM-FELIX-related appointments at the full professor level.
We are concerned that the FELIX director has left at a critical moment in this ambitious project. Urgent efforts are needed to appoint a new FELIX director, who should be a scientist of high profile within the SDM theme and who will, with the aid of colleagues, provide a fresh scientific impulse for the light source. This is crucial for the future of IMM. We are surprised by the lack of involvement of any SDM faculty in the IMM Board. This may reflect losses of key leaders within SDM. Nevertheless, the appointment of the new FELIX director should be used not only to strengthen the leadership in FELIX and SDM but also to improve SDM participation within the IMM Board. We recommend that an SDM faculty member with strong leadership abilities be appointed to the IMM Board to represent important SDM issues (especially those related to FELIX) in the discussions of the IMM Board. Ideally, this would be the new FELIX director.

Within the SDM theme we are particularly impressed with the success of Van de Meerakker. The Institute is to be strongly complimented in being able to recruit such an excellent young scientist and provide him the environment to be so successful. It is a sign of vitality that such excellent young people are joining the faculty. The IMM should provide an attractive career path to Van de Meerakker to make sure that he prefers to stay at Nijmegen in the long run.

We compliment the SDM faculty on their initiative to begin research in surface chemistry and dynamics. This will be very challenging to sustain and to expand in the future. We recommend that the Institute consider a new appointment in experimental surface science and dynamics to complement existing expertise and prepare for Parker’s retirement. This would allow for long-term development in this field, which aspires to address problems of great complexity and societal relevance.

Finally, the Trace Gas Facility has been very successful in the past. While we understand that the focus on large-scale facilities such as FELIX and HFML requires down-sizing in other areas, we believe that the University should find a solution to further exploit the potential and societal relevance of the Trace Gas Facility, also after the retirement of Harren. We support the envisioned link to the medical school and recommend this to be pursued by the IMM and the University.

The Committee considers the viability of Theme 1 very good and, therefore, of category 2.
Recommendations for the programme

- The Parker and Harren positions should be retained for SDM-FELIX-related appointments at the full professor level in the near future.

- Urgent efforts are needed to appoint a new FELIX director, who should be a scientist of high profile within the SDM theme and who will, with the aid of colleagues, provide a fresh scientific impulse for the light source.

- An SDM faculty member with strong leadership abilities should be appointed to the IMM board to represent important SDM issues (especially those related to FELIX) in the discussions of the IMM Board. Ideally, this would be the new FELIX director.

- The Institute should consider a new appointment in experimental surface science and dynamics to complement existing expertise and prepare for Parker’s retirement.

- The Institute should implement mechanisms for retention of exceptionally successful home-grown scientists also after becoming Associate Professor.
4.2 **Theme: Molecular Life-like Systems**

Leader: N/A

Academic staff in 2014: 60.4 fte

Assessment:
- Research Quality: 1
- Societal Relevance: 1
- Viability: 2

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**Research Quality**

The committee was deeply impressed by the quality of the forward looking research that was conducted by the group consisting of 18 faculty members (6.5 FTE). We congratulate the group for its excellent publication record in highly ranked journals and the very well recognized accomplishments.

We were particularly impressed by the research in the fields of (1) synthetic motors exploiting creative ways and molecular designs to convert different forms of energy into motion, (2) the design and characterization of synthetic extracellular matrices that can serve as intriguing new model systems for basic research in biology as well as for various medical applications, and (3) their efforts in the development of drug delivery systems. Here they focus on the blood brain barrier which fits well with the university wide initiative on the Healthy Brain. The synthetic organic chemists thereby see themselves as driving forces at the centre of these activities.

Even though little was written up in the self-assessment, we heard good evidence that valuable connections have been made to the local medical community, thereby taking advantage of the unique setting of Nijmegen that the Medical Centre is located on the same campus, essentially next door to the IMM activities. This connection ensures that their technologies are developed in the context of significant medical challenges.

Finally and during our lab tour, we heard about exciting ongoing research by the Huck team where they entrap immune cells and circulating cancer cells into microdroplets. These microdroplets can serve as a beautiful research tool for the study of single cells and what they secrete, as well as an analytical tool for various diagnostic medical applications. Huck just founded a start-up company around the diagnostic theme.

The Committee considers the research quality of Theme 2 world leading and excellent and, therefore, of category 1.
Societal relevance
Given the internationally recognized quality of their research, it is not surprising that the Theme 2 members were very successful in competing for various National, European and international awards. Congrats to Wilson for receiving an ERC starting grant and to Huck and Nolte for receiving ERC advanced grants. In 2013, theme members initiated the Radboud Nanomedicine Alliance whereby the Board provided seed funds of 1M€ per year. Buydens founded the successful national PPP COAST (Comprehensive Analytical Sciences and Technology) through which already more than 5M€ in subsidies have been obtained for different IMM groups. Notable is also their involvement in the gravitation grant “Research Center for Functional Molecular Systems” that started in 2012 which gives stable financial support over 10 years upon renewal.

The Committee considers the societal relevance of Theme 2 world leading and excellent and, therefore, of category 1.

Viability
An impressive number of eight spin-offs emerged from this theme, mostly spun out by the former graduate students of Rutjes. Rutjes was named the most entrepreneurial scientist of the Netherlands in 2008. Despite this success, the members of this theme emphasized the importance of basic science to their efforts and that they enjoy to research fundamental questions.

The Committee considers the viability of Theme 2 very good and, therefore, of category 2.

Recommendations for the programme
• Given the unique strength of the facilities in Nijmegen, the committee encourages the investigators of this theme to explore how they could take better advantage of FELIX. There are even ongoing research themes where we felt that the available facilities could be utilized to perhaps understand the underpinning mechanisms of the phenomena which they have discovered, for example the effect of crowding and confinement on supramolecular assembly and catalytic reactions.

• Even though analytics is an essential pillar of Theme 2, the high resolution NMR chair position could not be filled during the last few years. We heard that the group is now thinking of changing the focus onto another field in biophysical chemistry, perhaps towards super-
resolution microscopy. The feeling was that this would bring essential new expertise to IMM, while the NMR needs could still be covered by the senior researchers of IMM. Our committee strongly supports such discussions and the proposed reorientation.

- This is the only theme without theory, apart from the chemometrics research on big data, even though advances in atomistic molecular dynamics simulations of supramolecular assemblies make it possible today to give valuable guidance to the design of such systems and into the dynamics of their performance (see for example the Klaus Schulten group for the state of the art). The administration should perhaps consider giving IMM a new faculty position to address this need.
4.3 Theme: Quantum Matter

Leader: N/A

Academic staff in 2014: 41.5 fte

Assessment:
- Research Quality: 1
- Societal Relevance: 1
- Viability: 1

Research Quality

The committee was very impressed with the outstanding research activities on the “Quantum Matter” theme and the very well defined and synergic strategies for the next six years. In particular, the investigation of ultrafast magnetic phenomena and the study of novel electronic and magnetic phases in superconducting systems are the main leading activities, and they largely surpass the international standards.

Furthermore, the theoretical and experimental activities on 2D materials, such as graphene and beyond, have produced very important breakthroughs in the understanding of the physical properties of such emerging materials. In particular, the pioneering theoretical activities on hybrid van der Waals heterostructures have demonstrated the very unusual structural and mechanical properties of such innovative materials. The theoretical solid state activities are excellent by all standards: they are based on density functional theory, with appropriate refinements for electronically challenging systems (e.g., dynamic mean field theory, dual boson approach). The contributions from the theoretical solid state group are outstanding, both in terms of method development to understand complex physical phenomena, and in terms of collaborative cutting-edge applications together with experimental groups reflected by a large number of common papers. The theoretical activities on 2D materials are embedded in collaboration with the Nobel Prize winner Kostya Novoselov of Manchester University, who holds an extraordinary chair at IMM.

Moreover, the committee was impressed by the new scanning probe microscopy laboratory and in particular by the development of a new spin polarized STM, which operates at very low temperature (30 mK) and with vector magnetic fields. This activity is carried out thanks to the expertise of Alex Khajetoorians, recently appointed at IMM.

The excellence of the activities on the theme “Quantum Matter” is also reflected by the large number of publications, especially in journals with high impact factor, and a large number of citations. Another measure of the excellent success of the activities of this theme is the ability
to attract research funds in highly competitive national and European calls, such as ERC Advanced Grants or the Spinoza prize.

The Committee considers the research quality of Theme 3 world leading and excellent and, therefore, of category 1.

**Societal relevance**

The increasing number of collaborations with companies is strongly appreciated, especially due to the fact that the activities of this theme are mostly associated to basic research. Collaborations with the private sector via joined projects with large companies as well as small SMEs are established. Furthermore, the development of state of the art equipment in collaboration with companies and the establishment of Nanolab Nijmegen and SPIN laboratories is an important opportunity to provide expertise and infrastructure in the nanotechnology field to SMEs. In a more general context, the fundamental research within this theme may give rise to real breakthroughs in the field of quantum matter, which may be game-changing and trigger completely new industrial activities that go beyond of what can be envisioned today.

The Committee considers the societal relevance of Theme 3 world leading and excellent and, therefore, of category 1.

**Viability**

Viability is another strong point of this theme due to the excellent use of the international and unique facilities available in the IMM, such as the High Field Magnet Laboratory (HFML) and free electron laser facility (FELIX). In particular, the Quantum Matter groups are strongly involved in the operation of the HFML laboratory and also in the development of state of the art equipment such as a magnet which provides extremely large magnetic fields up to 45 Tesla. In-house research programmes are also foreseeing experiments that combine FELIX radiation with HFML and ultra-low temperature STM measurements at very high magnetic fields.

The Committee considers the viability of Theme 3 world leading and excellent and, therefore, of category 1.
Recommendations for the programme

- Continue efforts towards valorizing the recent scientific breakthroughs in ultrafast magnetic phenomena.
- Keep possible joint projects with companies active in photonics-based storage devices on the radar.
4.4 **Theme: Materials Design**

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<tr>
<td></td>
<td>Viability : 3</td>
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**Research Quality**

The committee supports the overall goal of Theme 4, namely, “The fundamental understanding of the structure - property relationship to design materials with novel functionality”. This is an excellent and worthy goal. The committee was impressed by the quality of the research that was conducted by the research groups assembled in the “Thematic Group 4: Materials Design”, over the past six years. The publication record in highly ranked journals is very good and other accomplishments are also well recognized. The committee is very much in support of the stated goals of this theme, namely the fundamental understanding of structure-property relationships and the design of materials with novel functionalities. We appreciate the excellent work that was presented to us and the effort of the thematic group to bring together more interdisciplinary research areas across IMM. Two interesting examples included world-leading efficiencies of GaAs-based solar cells and the forming of crystals of a given chirality from initial mixtures of both chiralities via rotational flow.

Overall, the committee is of the opinion that there could be more coherence between the research activities within the theme “Materials Design”. Also, it did not become clear to us how the theme is moving towards meeting the stated objectives. The Materials Design (MD) theme is presented as the heart of IMM with the argument that there is collaboration with all other themes and use of almost all different research facilities. The committee, on the contrary, feels that the broad approach is masking its core identity and may even endanger its existence as a separate theme.

The committee would like to wish Alan Rowan much success in his new position in Australia that reflects his very significant research contributions in the IMM over the past years. The committee recommends that the search for a successor to Alan Rowan provides an opportunity to refocus the theme and provide coherence to allow it to meet its stated objectives. Materials design needs an integrated programme encompassing: theory- namely the development of models and algorithms to allow for the calculation of particular properties,
as well as large scale computational calculations of designed materials, that are coupled to clear-cut experiments to develop novel materials and to validate the theoretical predictions.

The Committee considers the research quality of Theme 4 very good and, therefore, of category 2.

**Societal relevance**
The development of novel functional smart materials is by its nature of high relevance to society. As groups within the MD theme have been successful at producing novel functional materials, the societal aspects of their research are indisputably strong. The committee was glad to see that the Materials Design Theme has strong collaborations with the pharmaceutical, chemical, and semiconductor industry. Several of those partners have developed IP from their research resulting in a variety of patents and spin-offs. The committee appreciated the significant valorization of this theme with significant numbers of patents (12), public-private projects (13) and spin-offs (4).

The Committee considers the societal relevance of Theme 4 very good and, therefore, of category 2.

**Viability**
The committee sees in the new young hires who have been recognized with substantial awards (Elemans and Cuppen), the promise of a bright future for both MD and IMM. We value the appointment of a full professor in the theoretical chemistry cluster (Groenenboom) and also in the SCMN group (Christianen) which increases the collaboration with the HFLM facility. MD is exemplary for the collaborative environment at IMM by providing theoretical chemistry support to other themes, in particular to “Structure and Dynamics of Molecules” and by developing techniques to determine the mechanical properties of two dimensional systems in collaboration with the condensed matter theory of “Quantum Matter”.

Furthermore, the committee feels that the stated objective of understanding the dynamical process of nucleation and hierarchical assembly of complex materials is laudable and feasible. The proposed use of XFEL-radiation for the imaging of nucleation processes across a wide range of time and length scales is very interesting, and a roadmap should be provided on how to proceed in this direction during the next few years.

Finally, the NMR group has been instrumental in developing new technologies and approaches for studying molecular assemblies in the past. Still, the committee felt that the
NMR facility was not well enough integrated in the themes. It was also not clear which specific goals and projects IMM envisions in order to move the NMR facility forward in the coming six years.

The Committee considers the viability of Theme 4 good and, therefore, of category 3.

Recommendations for the programme

The departure of Alan Rowan to Australia is a disruptive event for the MD theme and a major loss. The committee recommends that the search for his successor be used as an opportunity to refocus the theme and to provide more coherence to allow the theme to fully meet its stated objectives. Materials Design has the potential to accelerate the discovery of materials with needed functionalities that could address several pressing problems that affect humanity on a global scale, as well as addressing fundamental scientific challenges. The committee recommends that the theme define a set of ambitious but well defined objectives that should be met over the next 6 year period coupled with a detailed roadmap that would allow for these objectives to be realized. This roadmap includes the hiring of a successor to Alan Rowan as well as the definition of theoretical and experimental tools that will be needed to meet these objectives. For example, the use of XFEL to follow the dynamics of nucleation processes that was proposed is a very interesting proposal but this will require a focused effort over a period of years to have a chance of success. The committee recommends that other potential techniques should be identified and paths to their development for this purpose be undertaken. It's unlikely that one technique could probe nucleation processes over all the needed spatial and temporal scales. Techniques in other themes could be adapted for this purpose. One technique mentioned by the theme, namely, liquid TEM seems attractive but will likely require the development of sophisticated double-tilt sample holders and even new microscopes with larger sample volume spaces within the objective lens pole pieces. 3D tomographic imaging techniques using electron or photon sources on appropriate time-scales could be of interest.
5. **Response of the institute**

The IMM Board thanks the committee for their careful and critical evaluation of our institute, the many positive remarks about the quality of the research and infrastructure and for the various suggestions and recommendations. We would like to use this opportunity to respond to a number of the most essential comments and recommendations regarding the institute as a whole and its individual Themes:

**Research infrastructure and facilities**

1) The committee mentioned in their evaluation that they would have liked to see a strategic plan for FELIX in the IMM’s self-evaluation report. We regret the absence of this plan in the documents. Meanwhile, FELIX has produced a concept strategy plan towards a roadmap application which was positively received by the "Permanente commissie Grootschalige Wetenschappelijke Infrastructuur" on April 8th 2016 and subsequently to a position on the Roadmap. For the vacant chair we will appoint a candidate in condensed matter science. In addition, new plans are developed in the existing biomolecular activities to strengthen the interactions with the research theme Chemistry and Spectroscopy of Complex Molecular Systems (theme 2).

2) Regarding NMR: Unlike the review committee, we do not feel that the complete NMR field is losing momentum. We believe that the solid state NMR is well embedded and well equipped within the national facility uNMRnl. We therefore plan to focus our efforts in that direction. The vacant chair will be used to strengthen our physical chemistry.

**Organization**

3) In the new IMM board, all current themes are represented.

4) We will split the position of scientific director of FELIX in a scientific position (in the field of condensed matter science) and a facility director. The facility director will act as the chairman of the FELIX board.

**Resources / Societal Relevance**

5) Regarding long term funding of our facilities: these are indeed a central and integral part of the IMM and we share the concern of the committee to safeguard their future. With the strong support of the dean of the Faculty of Science and the president of Radboud University, IMM, HFML and FELIX are currently exploring the possibility of getting the joint HFML/FELIX facilities recognized as a national facility within Radboud University under the wings of the National Science Foundation (NWO) whilst preserving their strong scientific embedding within the IMM.

6) We are developing a strategy plan for the next 6 years that includes how to become more successful in the valorisation/utilization of our research. This will further enhance the societal relevance of the IMM research.
7) Regarding human resources: we will use active scouting and the Christine Mohrmann program to increase the number of female professors and give exceptional talents (tenure trackers) more possibilities to grow to full professorship.

8) Regarding valorisation: with its focus on fundamental research on molecules and materials, valorisation of IMM research should be based on the research within its Themes and is primarily sought in Industrial Partnership programmes and the creation of spin-off activities where possible. Regarding the latter we feel that these should become independent as soon as possible, but definitely within 5 years. The (partly) ownership of companies is an interesting suggestion but against university policies.

PhD programmes, training and supervision

9) Regarding our PhD training: we will start courses on entrepreneurship and scientific integrity and, according with the recommendations of a recent KNAW report, prepare our students better on an eventual career outside academia after their PhD.

10) We will start a PhD tutoring programme for our PhD students to coach them on issues related to an active career in science.

Assessments per programme

11) Regarding our Themes: we have decided that the IMM should focus on and strengthen three themes that are or have the potential to be world leading: 1) Structure and Dynamics of Molecules, 2) Chemistry and Spectroscopy of Complex Molecular Systems and 3) Quantum Matter. These themes are all represented in the new IMM board and are all grouped around and make use of our unique facilities (HFML, FELIX, NMR, SPM, Laser Facilities).

12) Regarding comments on the research theme Structure and Dynamics of Molecules (theme 1): the positions of Parker and Harren have been reallocated and will be used to strengthen the research with FELIX; two new groups will be started, one as a successor of Van der Zande with a focus on condensed matter research and one on the interaction of cold molecules with surfaces (Van de Meerakker); Cuppen has been appointed to the IMM board.

13) Regarding comments on the research theme Chemistry and Spectroscopy of Complex Molecular Systems (theme 2): the use of FELIX for studies of biomolecular systems and catalysis will be (further) developed; the “NMR” chair will be strategically filled in a Physical-Chemistry direction; Matthias Bickelhaupt (VU) has been appointed as an extra-ordinary professor for theory.

14) Regarding the research theme on Quantum Matter (theme 3): we have been able to secure EU Future and Emerging Technologies funding and applied for an ERC Proof of Concept for the valorisation of All-Optical Switching, both include interactions with companies.

15) Regarding the research theme on Materials Design (theme 4): as stated earlier, we have decided to focus our research on the three themes mentioned above.

On behalf of the IMM, Theo Rasing and Freya Senf, Director and Managing Director IMM
6. Appendices

APPENDIX 1 Short Curricula Vitae of the Evaluation Committee members

Prof. dr. em. J.F. van der Veen (Chair)
Friso van der Veen (1949), emeritus professor since May 2014, is the former Head of the Research Department of Synchrotron Radiation and Nanotechnology as well as Deputy Director at the Paul Scherrer Institute in Villigen, Switzerland.
He studied Physics at the University of Utrecht in The Netherlands and received his PhD in 1978 with a thesis on a surface science topic. After spending a year as postdoc at IBM Yorktown Heights, he joined the staff at the FOM-Institute for Atomic and Molecular Physics in Amsterdam in 1980. In 1997 he was appointed Full Professor at the Van der Waals-Zeeman Institute of the University of Amsterdam. In May 2000 he was appointed Professor of Experimental Physics at ETH-Zürich.
In 1998 he received the Prize in Science from the International Union for Vacuum Science, Technique and Applications (IUVSTA).
His research interests have been in the application of synchrotron X-ray scattering techniques for the study of the structural properties of solid-liquid interfaces and of confined fluid films, and in the development of instrumentation for large facilities.
He has (co-)authored more than 240 publications in peer-reviewed journals, receiving circa 8900 citations so far (h-index=54).

Dr. Q.B. Broxterman
Rinus Broxterman (1956) is Corporate Science Fellow, Chemistry & Catalysis, at Royal DSM, The Netherlands.
He studied Organic Chemistry at the University of Groningen in The Netherlands and received his PhD in 1985. He worked a few years in the Flavours & Fragrance industry (Quest Int) and joined DSM in 1988 as a research chemist. Since, he has risen through the ranks in R&D and was appointed Corporate Scientist “Route scouting – and selection” in 2002.
His key area of expertise is the identification and development of novel synthesis routes for molecular products, with an emphasis on “Green Chemistry”. His skills have been employed for a wide range of compounds such as agrochemicals, semi-synthetic antibiotics, the sweetener Aspartame, specialty & fine chemicals and, in particular, pharmaceutical ingredients and intermediates (e.g. enantiopure unnatural amino acids and small peptides).
He has had an active role in the spin-out Isobionics (biotech manufacturing of Flavor & Fragrance intermediates) since its foundation in 2008. He is also involved in the spin-out Enzypep, set up 2012, where he currently acts as Strategy Advisor. He represents DSM on several Top Sector Chemistry Program Committees and in the Master programme Bio-Based Materials (BMM) at the University of
Maastricht, location Chemelot. He also serves on the Advisory Council of the International Sustainable Chemistry Collaborative Centre (ISC3), an initiative of the German government managed by DECHHEMA. He was elected Fellow of the Royal Society of Chemistry (UK) in 2014. He has (co-)authored over 200 papers and more than 20 patent applications.

Prof. dr. S. P.P. Parkin

Stuart Parkin (1955) is Alexander von Humboldt Professor at the Martin Luther University Halle-Wittenberg and Director of the Max Planck Institute of Microstructure Physics in Halle, Germany. He studied Physics and Theoretical Physics at Trinity College in Cambridge, United Kingdom, and finished his PhD in 1980 at the Cavendish Laboratory, also in Cambridge. He worked as Royal Society European Exchange Fellow at the Laboratoire de Physique des Solides, Université Paris-Sud, from 1980 to 1981. In 1983, after a year as IBM World Trade Fellow at the IBM Almaden Research Center in San Jose, California, he became a member of the Research Staff there. In 1999 he was named an IBM Fellow, IBM's highest technical honour. In 2004, when the IBM-Stanford Spintronic Science and Applications Center (SpinAps) was formed, he became its Director. In 2014, he became Director of the Max Planck Institute of Microstructure Physics in Halle, Germany. He was awarded an Alexander von Humboldt Professorship the same year.

He has received numerous honours and awards. He was elected Fellow of American Physical Society in 1992, Fellow of the Institute of Physics and of The Royal Society, London (UK), both in 2000; Fellow of the Institute of Electrical and Electronics Engineers (IEEE) (USA) and Fellow of American Association for the Advancement of Science (AAAS), both in 2003; Fellow of the Materials Research Society and Member of the National Academy of Sciences (USA), both in 2008; Member of the National Academy of Engineering (USA) and Fellow of the American Academy of Arts and Sciences, both in 2009.; Honorary Fellow of the Indian Academy of Sciences and Fellow of The World Academy of Sciences; both in 2012, Honorary Fellow of Trinity College, Cambridge (UK), in 2014, and Member of the German National Academy of Sciences Leopoldina (Germany), in 2015. He is also a Fellow of the Cambridge Philosophical Society and the World Technology Network, and holds Honorary Doctorates from the RWTH Aachen University (2007), Eindhoven University of Technology (2008), University of Regensburg (2011) and Technische Universität Kaiserslautern (2013).

His other awards and prizes include the American Physical Society International New Materials Prize of 1994, the 1997 Hewlett-Packard Europhysics Prize, the 2000 Jack Raper Outstanding Technology Directions Award from the IEEE International Solid-State Circuits Conference, Research & Development Magazine’s 2001 Innovator of the Year Award, the 2004 Humboldt Research Award for Senior U S Scientists from the Alexander von Humboldt Foundation, the 2007 “No Boundaries” Award for Innovation by The Economist magazine, the 2008 IEEE Daniel E. Noble Award, the 2008 IBM Corporate Award, the 2009 Dresden Barkhausen Award, the 2009 IUPAP Magnetism Prize and Neel Medal, the 2012 Von Hippel Award from the Materials Research Society, the 2013 Swan Medal of the Institute of Physics.
(London), the 2014 Millennium Technology Prize from the Technology Academy Finland and a European Research Council Advanced Grant- SORBET (2015).

He is a pioneer in the science and application of spintronic materials and invented the spin-valve read head. This discovery was transformed into practical and cost-efficient technology for data storage, as is nowadays at the heart of every computing device.

He has (co-)authored over 400 publications in peer-reviewed journals (h-index=87) and holds over 100 patents.

Prof. L. Sorba

Lucia Sorba (1958) is Director of the Institute of Nanoscience of the National Research Council (CNR) in Pisa, Italy.

She studied Physics at the University of Rome "La Sapienza" (Italy) and received her PhD summa cum laude in 1983. She worked as a postdoctoral fellow at the Fritz Haber Institut of the Max Planck Society in Berlin, Germany, for two years before her appointment to CNR staff scientist in Rome in 1986 and at the TASC-INFM Laboratory in Trieste in 1988. From 1997 to 1999 she was a visiting scientist at the Walter Schottky Institute of the TU Munich in Garching, Germany, supported by a Fellowship from the Alexander von Humboldt Foundation. Subsequently, she was appointed Associate Professor at the University of Modena (until 2006) and at the Scuola Normale Superiore in Pisa, Italy. In 2009 she became Research Director of the National Research Council at the CrS Nano NEST in Pisa and she has been Director of the Institute of Nanoscience since it was established in 2010.

Her research interests are in the field of experimental semiconductor physics and materials science. Mainly:

- Synthesis by molecular beam epitaxy and chemical beam epitaxy of III-V materials
- Magneto-transport properties of two dimensional electron gases in AlGaAs/GaAs and InAlAs/InGaAs systems
- Scattering mechanisms, morphological and structural, of InAlAs/InGaAs heterostructures.
- Chemical and morphological studies of nanostructures fabricated by local anodic oxidation technique
- Chemical composition study of self-assembled InAs-GaAs QD and QR
- Catalyst-assisted growth, transport and structural properties of semiconductor nanowires

To date, she has over 365 papers in peer-reviewed international journals, receiving over 3940 citations (h-index=32).
**Prof. dr. W. Thiel**

Walter Thiel (1949) is Director of the Theory Department at the Max-Planck-Institut für Kohlenforschung in Mülheim, Germany, and Honorary Professor at the University of Düsseldorf.

He studied chemistry at the University of Marburg, Germany, and received his PhD in 1973. After working as a postdoctoral fellow at the University of Texas at Austin, USA, until 1975, he returned to Marburg where he gained his habilitation in 1981. In 1983, he was appointed Associate Professor at the University of Wuppertal, Germany, and, in 1992, Full Professor at the University of Zürich, Switzerland. In 1999, he accepted the offer to become Director at the Max-Planck-Institut für Kohlenforschung in Mülheim, Germany. He has been Honorary Professor at the University of Düsseldorf since 2001.

His honours and awards include a Heisenberg Fellowship of the German Research Foundation (1982), the Förderpreis of the Alfried Krupp von Bohlen und Halbach Foundation (1988), the Schrödinger Medal of the World Association of Theoretical and Computational Chemists (2002), the Liebig Medal of the German Chemical Society (2012), and an ERC Advanced Grant (2013).

He was elected Member of the International Academy of Quantum Molecular Science and of the German National Academy Leopoldina, both in 2007. He has been President of the World Association of Theoretical and Computational Chemists since 2011 and belongs to the Board of Governors of the German Chemical Society since 2012.

His research interests include the development of theoretical methods and computer programmes, in particular combined quantum mechanics/molecular mechanics (QM/MM) methods and semi-empirical quantum-chemical methods for the treatment of large molecules. His computational studies cover a broad range of applications, often in cooperation with experimentalists, including:

- Highly accurate ab initio calculations on the spectroscopy of small molecules.
- Density functional studies on transition-metal catalysis.
- QM/MM investigations of enzymatic reactions and biocatalysis.
- Nonadiabatic simulations of the dynamics of electronically excited states.

He has (co-)authored over 550 publications, receiving over 30000 citations (h-index =75).

**Prof. dr. V. Vogel**

Viola Vogel (1959) is Head of the Laboratory of Applied Mechanobiology and Professor in the Department Health Sciences and Technology (D-HEST) at the ETH Zürich, Switzerland.

After completing her graduate research at the Max-Planck Institute for Biophysical Chemistry, she received her PhD in Physics at the Johann-Wolfgang Goethe University in Frankfurt/Main. She completed two years as a postdoctoral fellow at the University of California Berkeley, Department of Physics. In 1991, she became Assistant Professor in Bioengineering at the University of Washington/ Seattle, with an Adjunct appointment in Physics. She launched a new programme in Molecular Bioengineering, and was later promoted to Associate (1997) and Full Professor (2002). She was the Founding Director of the Center for Nanotechnology at the University of Washington (1997-2003) In 2004 she moved to the ETH in Zürich, Switzerland.
Her work has been internationally recognized by multiple awards, including Otto-Hahn Medal, NIH FIRST Award, Philip Morris Foundation Research Award, Julius Springer Prize 2006 for Applied Physics, ERC Advanced Grant (2008), major lectureships (including the Lacey Lectureship at CalTech in 2007), the Timoshenko Lectures at Stanford University (2011), the International Solvay Chair in Chemistry Brussels (2012), and an Honorary Doctorate from the University of Tampere Finland (2012). She served as the US Representative on the Council of Scientists of the Human Frontier Science Program, as well as a Jury member for the Queen Elizabeth Prize for Engineering, the European Research Council, the British Marshall Fund, the Humboldt Foundation, the National Research Council (USA); NASA, NIH, NSF, DOE and the German Government (BMBF). She was also a member of the Gordon Research Conferences Selection and Scheduling Committee and of the PCAST subpanel that finalized the National Nanotech Initiative (White House). She currently serves on several scientific advisory boards, including the Wyss Institute at Harvard, the Max-Planck Institute for Colloids and Interfaces (Golm), the Institute of Bioengineering and Nanotechnology (Biopolis Singapore), the Nano-Initiative-Munich (DFG Excellence Cluster), the Fondation Pierre-Gilles de Gennes, and is a Member of the Hochschulrat (Board of Regents) of the Ludwig-Maximilians-Universität München.

Prof. dr. A.M. Wodtke

Alec Wodtke (1959) is Alexander von Humboldt Professor and Director of the Department of Dynamics at Surfaces at the Max Planck Institute for Biophysical Chemistry in Göttingen, Germany. He graduated magna cum laude with a major in chemistry from the University of Utah in 1981 and received his PhD in Physical Chemistry from the University of California at Berkeley in 1986. He worked as a postdoctoral fellow at the Max Planck Institute in Göttingen, Germany, before joining the faculty at University of California at Santa Barbara in 1988. He received tenure in 1993 and became Full Professor in 1996.

In 2003, he began serving as Chairman of the Department of Chemistry and Biochemistry at UCSB and shortly thereafter became Associate Director for the Institute for Quantum and Complex Dynamics. In 2005 he was appointed Director of the Partnership for International Research and Education. In 2010, he accepted the offer from the Max Planck Society for the Advancement of Science to become Director and Scientific Member of the Max Planck Institute for Biophysical Chemistry in Göttingen. He was awarded an Alexander von Humboldt Professorship the same year.

Among his other honours are a Presidential Young Investigator Award, an Alfred P. Sloan Research Fellowship, a Camille and Henry Dreyfus Teacher Scholar Award and an Alexander von Humboldt Research Award. He was elected Fellow of the American Association for the Advancement of Science in 2007 and Fellow of the American Physical Society in 2009.

His research programme focuses on developing a theoretical understanding concerning the elementary events important to interfacial energy transfer and surface chemistry. That will eventually become a tool to design new chemical technology including: heterogeneous (photo) catalysts, photovoltaics and fuel cells. He has (co-)authored over 180 publications in peer-reviewed journals.
APPENDIX 2: Programme of the Site Visit

Wednesday 18 November
16.00 Chair and secretary (only) committee meet for program, logistics and procedures
16.45 Welcome to all Committee members by RU president, dean, directors of IMM and Theme leaders.
18.00 Internal Committee Meeting and Dinner to prepare interviews and report

Thursday 19 November
09.00 Presentation on IMM (institute level) by director Prof. Elias Vlieg, followed by interview.
11.00 Interview Theme 1 ‘Structure & Dynamics of Molecules’
12.30 Lunch with PhD students
13.30 Interview Dean / Faculty Board
14.30 Interview Theme 2 ‘Molecular Life-like Systems’
16.00 Tours along facilities (chemistry and large facilities, including switch)
17.30 Committee wraps up first day and prepares second day
19.00 Dinner at ‘Heyendael Mansion’, room ‘Marijnen’ (on campus)

Friday 20 November
09.00 Interview Theme 3 ‘Quantum Matter’
10.30 Interview Theme 4 ‘Materials Design’
12.00 Lunch with Tenure Trackers
13.00 Committee prepares presentation
15.00 Presentation of the preliminary findings by Committee Chair, attended by RU president
15.30 Committee meeting on details of preparing report
17.00 Informal meeting with staff IMM
18.00 End of site visit

From Saturday 21 November
Chair and secretary of the Committee prepare the report
Appendix 3
Quantitative data on the institute’s composition and financing

Composition over the past 5 years
Research staff FTE is the nominal time spent on research. FTE’s are calculated according to Prof/UHD/UD = 0.4; postdoc 0.9; PhD student = 0.75 FTE for research.

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<td>63</td>
<td>46.1</td>
<td>66</td>
<td>49.8</td>
</tr>
<tr>
<td>Visiting fellows</td>
<td>4</td>
<td>-</td>
<td>9</td>
<td>-</td>
<td>8</td>
<td>-</td>
</tr>
<tr>
<td><strong>Total staff</strong></td>
<td>254</td>
<td>157.6</td>
<td>279</td>
<td>161.8</td>
<td>309</td>
<td>181.8</td>
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</table>

Financing over the past 5 years

<table>
<thead>
<tr>
<th>Year</th>
<th>2009</th>
<th>2010</th>
<th>2011</th>
<th>2012</th>
<th>2013</th>
<th>2014</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Funding:</strong></td>
<td>fte</td>
<td>%</td>
<td>fte</td>
<td>%</td>
<td>fte</td>
<td>%</td>
</tr>
<tr>
<td>Direct funding</td>
<td>101</td>
<td>49</td>
<td>95</td>
<td>45</td>
<td>95</td>
<td>40</td>
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<tr>
<td>Research grants</td>
<td>63</td>
<td>30</td>
<td>65</td>
<td>31</td>
<td>70</td>
<td>30</td>
</tr>
<tr>
<td>Contractresearch</td>
<td>43</td>
<td>21</td>
<td>51</td>
<td>24</td>
<td>70</td>
<td>30</td>
</tr>
<tr>
<td>Other</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td><strong>Total funding</strong></td>
<td>206</td>
<td>100</td>
<td>211</td>
<td>100</td>
<td>235</td>
<td>100</td>
</tr>
<tr>
<td><strong>Expenditure:</strong></td>
<td>M€</td>
<td>%</td>
<td>M€</td>
<td>%</td>
<td>M€</td>
<td>%</td>
</tr>
<tr>
<td>Personnel costs</td>
<td>14.1</td>
<td>65</td>
<td>14.5</td>
<td>71</td>
<td>15.9</td>
<td>64</td>
</tr>
<tr>
<td>Other costs</td>
<td>7.5</td>
<td>35</td>
<td>6.0</td>
<td>29</td>
<td>8.8</td>
<td>36</td>
</tr>
<tr>
<td><strong>Total expenditure</strong></td>
<td>21.6</td>
<td>100</td>
<td>20.5</td>
<td>100</td>
<td>24.8</td>
<td>100</td>
</tr>
</tbody>
</table>
## Appendix 4
Explanation of the categories utilized

<table>
<thead>
<tr>
<th>Category</th>
<th>Meaning</th>
<th>Research quality</th>
<th>Relevance to society</th>
<th>Viability</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>World leading/</td>
<td>The research unit has been shown to be one of the few most influential research</td>
<td>The research unit makes an</td>
<td>The research unit is excellently equipped for the future.</td>
</tr>
<tr>
<td></td>
<td>excellent</td>
<td>groups in the world in its particular field.</td>
<td>outstanding contribution to society.</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Very good</td>
<td>The research unit conducts very good, internationally recognised research.</td>
<td>The research unit makes a very good</td>
<td>The research unit is very well equipped for the future.</td>
</tr>
<tr>
<td>3</td>
<td>Good</td>
<td>The research unit conducts good research.</td>
<td>The research unit makes a good</td>
<td>The research unit makes responsible strategic decisions and is therefore</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>contribution to society.</td>
<td>well equipped for the future.</td>
</tr>
<tr>
<td>4</td>
<td>Unsatisfactory</td>
<td>The research unit does not achieve satisfactory results in its field.</td>
<td>The research unit does not make a</td>
<td>The research unit is not adequately equipped for the future.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>satisfactory contribution to society.</td>
<td></td>
</tr>
</tbody>
</table>
Radboud University

Comeniuslaan 4
PO Box 9102
6500 HC Nijmegen
The Netherlands
Phone +31 (0) 24 361 1236
E-mail c.mollema@soo.ru.nl
Internet www.ru.nl