

**Research Assessment 2010-2015**  
**Leiden Institute of Chemistry**

**April 2017**

## **Preface**

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This evaluation report assesses the quality, societal relevance, viability, and other aspects of the research and educational activities of the Leiden Institute of Chemistry (LIC). It was commissioned by the Board of Directors of Leiden University as part of the regular quality control procedures established by the Association of Universities in the Netherlands (VNSU), the Netherlands Organization for Scientific Research (NWO), and Royal Netherlands Academy of Arts and Sciences (KNAW). The audit covers the period 2010 to 2015 and is a follow-up of a previous evaluation, which took place in 2011 by a committee that assessed all Chemistry departments in the Netherlands. The main purpose of this evaluation report is to give feedback on issues that are important for the future research and educational activities of the LIC. It is the result of constructive discussions between the director and staff of LIC and the committee members. The committee wants to thank all of them for the open and pleasant way in which this operation could take place.

April 2017

Prof. dr. Roeland Nolte, Chair

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## **The Evaluation Board and the review procedures**

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### **1. The System of Quality Assessment of Research in The Netherlands**

An external committee of peers (henceforth the 'Evaluation Board' or EB) evaluated the research quality of the Leiden Institute of Chemistry (LIC) during a site visit in February 2017, and reports its findings in this document.

This peer review is part of the assessment system for all publicly funded Dutch research organizations. In accordance with the Standard Evaluation Protocol 2015-2021 for Research Assessment in the Netherlands (SEP), the EB's task was to assess the quality and other aspects of the research of the LIC and its ten research groups on the basis of the written information provided by the Institute and the interviews with the management, research leaders, staff members, members of the PhD programme management and PhD students, as well as to advise on possible improvements.

### **2. Criteria and Assessment Scale**

The SEP requires the EB to assess the research according to three main criteria:

- Research quality (the level of the research conducted);
- Societal relevance (social, economic and cultural relevance of the research);
- Viability (strategy, governance and leadership).

The qualitative assessments are supplemented by assigning discrete categories (1-4): Excellent (1); Very good (2); Good (3); Unsatisfactory (4). Appendix 2 provides a complete description of each of the categories on this four-point scale.

### **3. The Members of the Evaluation Board**

The Evaluation Board consisted of:

Prof. dr. R. Nolte (Chair, Radboud University Nijmegen, the Netherlands);  
Prof. dr. A. Groß, Ulm University, Germany;  
Prof. dr. A. Llobet, Barcelona Institute of Science and Technology, Tarragona, Spain;  
Prof. dr. J. Jiménez-Barbero, CIC bioGUNE, Derio-Bizkaia, Spain;  
Prof. dr. E. Tate, Imperial College London, UK.

Dr. Jetje De Groof (Belgium) was appointed as secretary to the Evaluation Board (EB).

A short curriculum vitae of each of the members is included in Appendix 1.

All members of the EB signed a statement of independence to ensure that they would judge without bias, personal preference or personal interest, and that their judgment is made without undue influence from persons or parties committed to the institute or programmes under review, or from other stakeholders.

### **4. Scope of the Assessment**

The Leiden Institute of Chemistry (LIC) is one of the eight institutes of the Faculty of Science, which is one of the seven faculties of Leiden University. Over the past years the LIC has restructured itself around two major research areas: Chemical Biology and Energy & Sustainability. The LIC Chemical Biology research is conducted by seven research groups: the Bioorganic Synthesis (BIOSYN) group, the Macromolecular Biochemistry (MACBIO) group, the Metals in Catalysis, Biomimetics and Inorganic Chemistry (MCBIM) group (this group

participates in both research areas), the Supramolecular and Biomaterials Chemistry (SBC) group, the Medical Biochemistry (MBOC) group, the Biophysical Structural Chemistry (BSC) group, and the recently created Molecular Physiology (MOLPHYS) group. The LIC Energy & Sustainability research is conducted by four research groups, namely the Theoretical Chemistry (THEOR) group, the Metals in Catalysis, Biomimetics and Inorganic Chemistry (MCBIM) group (which also participates in the other focal area), the Biophysical Organic Chemistry (BPOC) group and the Catalysis and Surface Chemistry (CASC) group.

The current assessment includes the evaluation of the LIC and covers the period 2010-2015. The scope of the assessment is set by the Terms of Reference (TOR). According to the TOR, the EB is asked to judge the unit's performance on the three assessment criteria put forward in the SEP: research quality, relevance to society, and viability. In the SEP, indicators of research quality explicitly include such outputs as research articles, scientific books, Ph. D. theses, instruments, and infrastructure developed by the research unit. Important indicators are also number of citations of papers, science awards and scholarly prizes, invited lectures, memberships of scientific committees and editorial boards, the acquisition of individual research grants, etc. The relevance to society aspect involves research products for societal target groups with indicators such as policy making reports, outreach activities, projects in collaboration with societal parties, patents and licences, and valorisation funding. The viability assessment criterium includes amongst others the strategy that the unit intends to follow in the coming years with respect to research performance and societal relevance, and the extent to which the unit is capable of realizing its ambitions. Also the governance and leadership skills of its management should be rated.

At the level of the Institute, the EB is invited to provide a qualitative assessment and to also assign the research unit to a particular category (1: excellent, 2: very good, 3: good, or 4: satisfactory), in accordance with the SEP-criteria, taking into account current international trends in science and society. Furthermore, the EB is required to pay special attention to two aspects in its assessment: (1) the choice for the two major research areas: Chemical Biology and Energy & Sustainability and (2) the quality of the individual research groups. In accordance with the SEP, the EB is invited to reflect on the following three aspects in its report: (1) PhD programmes, (2) research integrity, (3) diversity. Finally, the EB's task is to formulate recommendations.

At the level of the individual research groups, the task of the EB is to discuss the 'quality of research', 'relevance to society' and 'viability' of each of the research groups. No grades are required.

#### **4. Data provided to the EB**

The EB members received a documentation package in advance of the site visit. This contained the self-evaluation of LIC and information on the individual research programmes, with a description of the mission, objectives and results achieved by LIC in the reporting period, as well as developments anticipated in the future. The documentation included quantitative data about staff composition, PhD's, publications, financial resources and, furthermore, information about societal output, a SWOT analysis, policies regarding research integrity, and the strategy for the future. The EB also received the SEP and TOR for its assessment.

#### **5. Procedures followed by the EB**

EB members were asked to read the complete information package and provide their preliminary appraisal of both LIC as a whole and the individual research groups prior to the site

visit. This was used as input for a preparatory meeting that was held on the night before the site visit.

The Chair of the EB assigned research groups to each EB member, taking into account their expertise. This enabled EB members to pay particular attention to their designated task areas during preparation and take the lead in interviews and discussions during the site visit as well as in the subsequent reporting.

Appendix 3 shows the programme of the site visit. Presentations, interviews and discussions on both the LIC level and with the individual research groups were held at the institute in Leiden. Between the interviews, time was available for the EB to discuss the various findings. During the last day of the site visit, a closed EB session was held so that all members could come to consensus on the final assessments of LIC and its research programmes. At the conclusion of the visit, the Chair orally presented the main preliminary conclusions of the EB to the staff and director of LIC. The Dean of the Faculty of Science, Prof. Dr. G. de Snoo, attended this meeting.

After the site visit, the evaluation report was prepared, with each EB member taking the lead in composing the sections they had focused on. An integrated version of the report was then circulated to the EB for comment. A final version, that took these comments into account, was then drawn up and sent to LIC for a check on possible factual errors. Finally, the report was delivered to the Executive Board of Leiden University.

## Leiden Institute of Chemistry (LIC)

**Assessment by the Evaluation Board:**

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

## **1. Description of the Leiden Institute of Chemistry (LIC)**

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The preparatory documents and the site visit gave the EB a clear view of the mission, structure and organization of LIC. A summary is given below.

### **1.1. Mission and research activities**

LIC's mission is to perform chemistry research and education at an internationally competitive level. Its strategy to achieve this is by providing an open and inclusive environment where curiosity-driven research can flourish and where research and education go hand in hand. Chemistry researchers at Leiden University, so the EB read in the preparatory documents and heard during the presentations by the director and the academic staff members, take a fundamental approach in finding tailored solutions for complex societal problems in human health and environmental issues.

LIC's research is organized around two major research areas: Chemical Biology and Energy & Sustainability. The LIC Chemical Biology research is aimed at understanding biological processes on a molecular level to strengthen the knowledge base of human health and disease. Its approach to achieve this goal is a fundamental chemical one: with the aid of chemical probes, biological systems are interrogated. In this way LIC researchers aim to contribute to the understanding of molecular mechanisms that are at the basis of human health and disease. LIC researchers also have the objective to develop agents and methodology through which the onset and progression of disease can be monitored in detail, as well as to contribute to the development of new therapeutic agents for unmet medical needs.

LIC research in the area of Energy & Sustainability is focused on obtaining fundamental understanding of chemical reactions of importance to the sustainable and efficient production of fuels and storage of chemical energy, and the subsequent usage of stored energy. Advanced spectroscopic techniques are employed as well as nano-imaging, inorganic synthesis, and theoretical methods to elucidate the molecular processes that are at the basis of the conversion of solar energy to chemical energy. In addition, new catalysts, materials, and molecular and supramolecular systems are developed and investigated. The ultimate aim is to make a fundamental contribution to a sustainable cyclic chemistry, which is efficient, scalable and robust.

### **1.2. Management and organization**

The LIC is the basis from which chemistry research groups at Leiden University perform their research activities. In 2011 both the report of the former research assessment and the Sectorplan Physics and Chemistry provided the starting point for a period of transition, allowing LIC's scope to change from a classical chemistry department that harbours 'all' chemical subdisciplines, into an institute that, based on its strengths embedded in the top-quality research groups (as acknowledged by the 2011 evaluation report), elaborates areas of focus related to important societal challenges. LIC activities were streamlined by restructuring the leading research groups into two focal areas, namely Chemical Biology and Energy & Sustainability. During this period of restructuring two research groups that were scored below par in the 2011 evaluation were discontinued, successful groups that are considered to be of pivotal importance to LIC's chosen profile were strengthened, and new groups were created (Supramolecular & Biomaterials Chemistry and Molecular Physiology). The EB read that the coming years will be devoted to expand the visibility of the Institute.

The Chemical Biology research is conducted by seven research groups: the Bioorganic Synthesis (BIOSYN) group, the Macromolecular Biochemistry (MACBIO) group, the Metals in Catalysis, Biomimetics and Inorganic Chemistry (MCBIM) group (this group participates in both research



areas), the Supramolecular and Biomaterials Chemistry (SBC) group, the Medical Biochemistry (MBOC) group, the Biophysical Structural Chemistry (BSC) group, and the recently created Molecular Physiology (MOLPHYS) group. The LIC Energy & Sustainability research is conducted by four research groups, namely the Theoretical Chemistry (THEOR) group, the Metals in Catalysis, Biomimetics and Inorganic Chemistry (MCBIM) group (which also participates in the other focal area), the Biophysical Organic Chemistry (BPOC) group and the Catalysis and Surface Chemistry (CASC) group.

Within the groups of the Chemical Biology cluster, a total of fourteen Principal Investigators (PIs) are active; the groups of the Energy & Sustainability clusters have nine PIs in total. All groups are led by a senior staff member (usually at the Full Professor level), and most groups host one or more Tenure Track PIs (at the Assistant Professor level or Associate Professor level). The groups are supported by expert support staff. They organize individual group meetings and monthly cluster seminars.

LIC's aim is to create an environment in which research can be conducted in a highly collaborative spirit, with intellectual freedom in terms of research directions taken by the LIC principal investigators, although collaborations between the groups are strongly stimulated.

LIC's management team consists of a Scientific Director (currently prof. dr. Jaap Brouwer), the Institute Manager (currently drs. Lian Olsthoorn-Tielemans), and two Educational Directors (currently prof. dr. Lies Bouwman and prof. dr. Mathieu Noteborn). The management team meets weekly on personnel and financial matters. The Institute's Research Council, which consists of all the PIs of the Institute, gathers on average every four weeks to discuss strategic research and educational matters. The LIC office also employs both a full time legal affairs (IP) and funding advisor, offering LIC staff support in setting up and maintaining international collaborations, in capitalizing on scientific findings and in the establishment of, or participation in, public-private partnerships.

LIC reports that its researchers maintain large national and international collaborative networks and contribute to the advancement of chemical sciences in individual projects, in academic (inter)national networks and by partaking in national and international public-private partnerships (PPP). This is an area in which LIC reportedly wants to take additional action in the years to come.

LIC researchers in the area of Energy & Sustainability are member of a large number of nation-wide consortia (among others the 'Towards Biosolar Cells Consortium' (TBSC), NanoNextNL, CATCHBIO). LIC reports that the researchers in this area collaborate with large and smaller industrial partners in consortia that have been successful in acquiring funding, both at the national and international level.

The LIC scientists of the cluster of Chemical Biology have established strong ties with researchers from Dutch Academic Medical centres (from both Leiden and elsewhere), the Dutch Cancer Institute, as well as researchers worldwide. Strong ties also exist with private partners. The Chemical Biology research cluster contributes to the Leiden University research themes of 'Bioscience: the Science Base of Health' and 'Translational Drug Discovery and Development'. Researchers from the cluster are partner of the European Lead Factory and were one of the partners establishing the national cancer Drug Discovery Initiative. Also, they were one of the partners establishing the Institute for Chemical Immunology, funded by the Gravitation Program ('Zwaartekracht programma').

### **1.3. Graduate education**

With the establishment of the LIC research areas of Chemical Biology and Energy & Sustainability, education at the master level has also been adapted. The Msc Chemistry track in Chemical Biology was revised and a track Energy & Sustainability was introduced. A 'Netherlands Research School of Chemical Biology' was created, together with researchers from

other universities (Eindhoven, Nijmegen, and Groningen), and acts as the National Graduate School for the Chemical Biology cluster. In this graduate school tailored training for talented master students and PhD students is offered. The Energy & Sustainability area is part of three inter-university research schools, namely the Netherlands Institute for Catalysis Research (NIOK), the Netherlands' Magnetic Resonance Research School (NMARRS) and the Holland Research School of Molecular Chemistry (HRSMC). These three research schools also have an NWO-funded graduate school, in which the CASC, BPOC and MCBIM groups participate. These research and graduate schools give MSc and PhD students of the LIC access to high-level specialized courses organized by HRSMC, NIOK and NMARRS.

## **1.4. Resources**

### **1.4.1. Human Resources**

Appendix 4, table 1 shows an overview of the composition of LIC staff. Over the evaluated period the staff of the LIC has grown from 223 to 297 members (179.4 fte to 234.2 fte). The table shows that this growth is caused almost completely by the increased number of PhD students, the number of which has risen from 89 in 2010 to 159 in 2015 (74.7 fte to 123.7 fte). In this period, the number of scientific staff rose from 39 to 47 (36.4 fte to 41.1 fte) and the postdocs from 45 to 47 (31.4 to 34.2 fte).

LIC reports that it considers the tenure track system to have been an important instrument in its human resources policy. The system gives young researchers the chance to develop their own independent research group while profiting from the experience of the established senior researchers that are already present. At the same time, the system allowed LIC to fill gaps between expertises of the established groups and to strengthen their positions. It also brought three (out of ten) new researchers from abroad, making the Institute's composition more international.

Currently, less than 10% of LIC's full professors are female (see graph in Appendix 9; in fact this is only one out of thirteen full professors). Progress has been made in recent years at the level of undergraduate and graduate students, and with the appointment of three female tenure track staff members. LIC stresses that attracting more female researchers is a priority for the future and observes that this problem is indeed the same for all institutes in the Netherlands and in surrounding countries.

Appendix 4, Chart 1 shows the Institute's age distribution. LIC mentions that the current distribution guarantees that successors for staff members that will soon retire are in principle already present in the Institute.

### **1.4.2. Financial resources**

LIC's sources of funding are presented in Appendix 4 (Table 2 and Chart 3), which shows that the portion of LIC's direct funding has decreased from 46.8% in 2010 to 40.6% in 2015, but when this data is added to the Sectorplan funding (0.4% in 2012 and 6.8% in 2015) and the funding obtained via the Gravity programme (0.1 % in 2014 and 1.4% in 2015) it can be concluded that the overall direct funding has remained more or less constant (~45%). The contribution of national research grants (NWO, STW, FOM, and KNAW) to the total funding has fallen from 39.6% in 2010 to 29.1% in 2015. On the other hand, the portion of EU research grants has risen from 6.9% in 2010 to 15.4% in 2015, making that the total funding via National and EU research grants has also remained stable over the assessment period. The income from contract research did not vary much either: it remained stable at 6.7% of the total funding. LIC reports that in 2015 47% of its budget was derived from competitive sources in spite of growing competition. The institute explains that both senior and junior staff members have been

successful in NWO (Top/Echo, VENI/VIDI/VICI) and EU (ERC) personal grant schemes. Also, they have been successful in establishing collaborations with industry, either in public-private partnerships or as direct collaborations. In addition (though on a more incidental basis) LIC researchers are partners in successful large program grant applications.

LIC's financial policy starts from the basis that each PI has full responsibility for external funding acquired by her/him and has full authority to recruit PhD students and postdocs funded by their own budget. The LIC provides each PI with a consumables budget from university sources based on the number of people in her/his group. The Institute moreover provides finances for hiring PhD students for specific purposes such as start-up packages for tenure track PI's. Occasionally, the Institute offers funding for hiring a PhD student in the case an A+/A rated proposal in the open national competitions was not granted by the subsidising agency.

### 1.4.3. Infrastructure

The Institute recently moved to a brand-new laboratory building - shared with the Leiden Academic Centre for Drug Research (LACDR), designed to support collaboration and to provide an open structure to its undergraduate students.

Infrastructure managed by the Chemical Biology focal area includes, besides instrumentation inherent to the research practice of the individual research groups, the Paramagnetic NMR Facility (a nationwide infrastructure tied to the MACBIO and BIOSYN groups) and the Chemical Proteomics Facility (tied to the BIOSYN group). The LIC took the initiative for the formation of a Faculty-wide infrastructure termed Cell Observatory in which researchers from LIC, LACDR, the Institute of Biology Leiden (IBL) and the Leiden Institute of Physics (LION) collaborate. The Cell Observatory houses a number of shared facilities for life sciences research including a Zebrafish Facility, advanced microscopes, and tissue culture facilities. Furthermore, there is a facility for cloning and protein purification as well as for protein crystallisation and X-ray structure determination.

The Energy & Sustainability researchers are supported by state-of-the-art infrastructure including instrumentation for solid state NMR, a multitude of state-of-the-art atomic- and molecular-level spectroscopic and imaging techniques, and access to infrastructure with large computational power.

## 2. Assessment of Leiden Institute of Chemistry

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In this section, the EB evaluates the performance of the LIC as a whole based on the three SEP criteria of research quality, relevance to society and viability. In addition, the EB gives its evaluation of PhD supervision and education, research integrity, and diversity, as stipulated in the TOR. An overview of the EB's recommendations is given in section 3 of this report.

### 2.1. Research quality

The EB noticed from the documentation and the presentations of the director and scientific staff members, as summarized in the chapter "Description of LIC" of this report, that the Institute has undergone a major reorganization in the period covering this assessment. The Faculty of Science in Leiden has chosen for disciplinary institutes with coherent and content-driven topics, rather than for classical Schools or Subfaculties with as a result that for LIC research and education are concentrated on Chemistry. Within the broad field of Chemistry there are many possibilities for carrying out challenging research, but it was decided to bundle the activities around the clusters Chemical Biology and Energy & Sustainability. The EB is pleased with this decision, which was made by the Institute itself, because it builds upon the former and current strengths of the groups participating in LIC, also taking into account the focus areas selected by Leiden University. The PI's seem to be happy with both the choice for a disciplinary institute and the selection of the two particular research themes, as was concluded from the discussions with the staff during the site visit. Furthermore, the chosen themes mean that the Institute can more easily respond to the current, stronger call for higher societal relevance of university research.

The quality of the research in both the Chemical Biology and Energy & Sustainability themes is excellent and world leading. The EB very much appreciates the science-driven attitude and atmosphere within LIC, which is also attractive for scientists, including professors, from outside The Netherlands. The research talks given by the PI's during the site visit and the (selection of) scientific highlights presented in the Self-assessment report revealed many exciting breakthroughs, both for the Chemical Biology and the Energy & Sustainability cluster, validating this conclusion. Many of the papers were published in highly ranked international journals, such as JACS, Angewandte Chemie, Nature Chemistry, Nature Communications, PNAS, and PRL, which is excellent. The number of publications and books/book chapters varied between ca. 160 and 190 per year over the period of the assessment, with roughly equal contributions by each of the two research themes (Table 3, Appendix 3). These publications are very well cited according to the survey carried out by the Dutch Institute for Bibliographic Analysis, mentioned in the Self-assessment report and given to the EB as a separate document. This bibliographic analysis revealed that the average number of citations, which LIC papers received compared to the average for its field of research, amounted to 1.79, which is much higher than the world average (set to 1.00).

The number of Ph. D. theses per year, being an important scientific indicator, is high and rather constant, i.e. around 17 (Table 4, Appendix 4), which is an excellent score. It can be expected that this figure will drastically increase in the future as a result of the growth of the number of Ph.D. students in recent years (cohort 2011-2015 encompasses 161 students, compared to 91 for the cohort 2006-2010; Appendix 4, Chart 4), which is very positive.

The funding acquired by the various groups of LIC is substantial (see Chapter 1.4.2 of this report). It includes a large number of grants from NWO, ERC grants (including prestigious ERC Advanced Grants), and grants from industrial or related sources. The overall funding of the institute has increased from 173 to 215 FTE, which is very positive. It is composed of ca. 45% direct funding, ca. 45 % funding by National and EU institutions, and ca. 10% funding from contract research (see Chapter 1.4.2 of this report). The latter number is relatively low given the

foreseen societal relevance of the two research themes, but it may increase in the future when these themes have taken further shape.

Based on the number of invited and plenary lectures the EB concludes that the group leaders are active in presenting the results of their research activities at conferences and meetings. This is important in order to make the institute known to the scientific community. In that respect it is also positive that many of the PI's are members of the Boards and Advisory Boards of Scientific journals. Several PI's have been awarded prizes, which is an important element of recognition of research quality.

The Institute's researchers are linked to many national and international collaborative networks and have strong ties with academic medical centers. They contribute to research themes of other institutes in Leiden and in The Netherlands and often take a leading role, which is a very positive attitude.

The infrastructure of LIC is excellent. The committee EB visited the new research labs and concludes that they are superb. These facilities surely will boost the research activities of LIC in the near future.

The organization of LIC seems well optimized and adequate to achieve the formulated goals of the Institute and the two research clusters. The management board works efficiently and the Institute's Research Council gives proper feedback on strategic matters. The director Prof. Brouwer runs the Institute very competently and has done great work in remodelling LIC and bringing it to its current format. He has monthly meetings with the scientific directors of other institutes of the Faculty of Science to exchange ideas and increase the interactions between the institutes. The same holds for the Managing Director who regularly meets with other Managing directors. The EB feels that in the future the Institute should formally appoint leaders to each of the two research areas, who might also become members of the LIC management team, which now has two Educational Directors and only one Scientific Director, who is no longer active in research.

***Taking all above mentioned indicators (quality and number of papers, Ph.D. theses, funding, organization, etc.) into account the EB considers that the aspect Research Quality should be rated as 1 (excellent/world leading).***

## **2.2. Relevance to society**

As mentioned above the EB is very positive about the major rearrangement of the structure of LIC, which has taken place in the past period. The two chosen research themes are highly relevant and very important for society and industry. Chemical Biology's objectives to study and understand the molecular aspects of human health and diseases as well as to develop new methodologies to monitor medical disorders and new therapeutics to treat them, are of the utmost importance and an outstanding contribution to society. The same holds for the formulated targets of the Energy & Sustainability cluster. The environmentally friendly production, storage, and efficient usage of energy are together one of the most important goals (goal 7) of the United Nations Sustainable Development Programme. The latter cluster with its focus on catalysis, solar energy conversion, and new (supra) molecular materials is well equipped to make an outstanding contribution to this international programme. Both research themes are in line with the National Research Agenda in The Netherlands.

Having said this, the EB feels that the two themes should be further defined and focussed. What are the overarching ambitions of the clusters and how can these be realized? What specific (fundamental) problems might be solved and what knowledge should be gathered in the coming

years? Such questions are currently not fully answered. In this connection also valorization indicators are needed. These have to be developed by the institute. The number of patents of the institute, which is very good, is just one indicator; importantly, this success in filing patents should be converted more frequently into societal and economic impact through licensing and spin-out companies in the future. The number of trained Ph.D. students is another one, but more are required. The EB would like to stress that, following up on its discussions with the staff, the extent to which the Institute is focussed on basic curiosity driven research is also a valorization indicator, and a positive one. This type of research should certainly remain the prime mission of the researchers of LIC, because it provides fundamental insight and leads to new discoveries, which in the end serves society best. This aspect of academic work surely falls under the heading Societal Relevance, but is nowadays increasingly not appreciated or even ignored (see also below).

The outreach activities of LIC are extensive and excellent, but according to the Self-assessment report mainly focused on high school students, which by itself is fine. One might consider, however, to give more attention to the teachers of these high school students, instead of to the students themselves. If teachers are motivated, the students will follow as well.

The collaboration with societal organizations (medical centers and industry) is very good, but there is room for further improvement, as can be noted from the fact that only 10% of the institute's funding comes from contract research (see also paragraph 2.1 above). It is not clear to the EB what the concrete goals of LIC are. Contract research reportedly is on the rise and increased visibility, as achieved through clustering in a research theme, is considered to be an important facilitator to acquire more funding from this type of research. With respect to patenting it can be concluded that some groups are more active than other groups. The appointment of a support officer by LIC is a very good move and is much appreciated by the staff. Spinoff companies are important for the transfer of knowledge from academia to society. It can be seen that some groups are more inclined to start a spinoff than others, because the latter "just want to do (fundamental) science". Perhaps, the idea of an entrepreneur in residence is worth considering to facilitate the creation of spinoffs. A further discussion of these aspects of societal relevance by the LIC and more guidance by the management is recommended. The EB encourages LIC to define more focal areas for public-private partnerships, spinoffs, and related valorization activities, because the funding landscape in The Netherlands is currently changing, i.e. away from fully independent, curiosity driven research and, unfortunately, most likely not in a reversible way.

***Altogether, the EB concludes that the institute is very much on the right track with respect to the assessment element Societal Relevance and considers that this aspect can be rated 1-2 (very good to outstanding contribution to society).***

### **2.3. Viability**

Given the size of LIC, the choice to maintain two general research themes is wise. These two themes are currently unbalanced: six are part of the Chemical Biology cluster and three of the cluster Energy & Sustainability (the EB did not receive numbers on the total amount of fte's staff in each of the clusters). One group (MCBIM) belongs to two themes. It is not clear to the EB what precisely defines a group. Is the wish or need for independence of a PI a starting point for a group? According to the discussions with the staff this seems to be the case. A better and more clear strategy is needed here.

In order to be sufficiently strong and viable a size of six to seven groups is more or less required. The Chemical Biology cluster has this size, but some individual groups (e.g. MOLPHYS and BSC)

are too small to have a large impact. This may require some re-thinking and probably reshuffling of staff or addition of expert support staff. The research programmes of the various groups of Chemical Biology are excellent, but the overall coherence of the cluster should be improved: there is as yet no overarching research theme, as was also mentioned in the Self-evaluation report. The EB recommends to work on this aspect because it will help increase the visibility of the cluster on the international scene. The addition of the Medicinal Biochemistry group to the cluster as a linking pin is a very good idea. More such actions would be welcomed.

The EB feels that the Energy & Sustainability cluster is too small and should be expanded, either directly by the addition of groups or by setting up stronger collaborations with groups from other institutes in Leiden or even other universities in The Netherlands, e.g. Delft. The cluster already refers to a number of national and international interactions in the Self-evaluation report, but given the fact that it has such a coherent and challenging overarching theme the societal impact may remain too low if a further strong effort in this direction is not made. At the moment, the cluster does not reach the critical size to have a significant and long-lasting impact in the competitive field Energy & Sustainability that is addressed by many strong groups and consortia around the world.

LIC has one group that acts as a bridging group between the Chemical Biology and Energy & Sustainability clusters. Such a bridging position is very demanding and requires a clear vision, both from the Institute and the group, as to where one wants to go. In general, the question regarding the need and role of bridging groups (linking pins) between the two clusters should be discussed further and a better strategy developed.

The Faculty of Science in Leiden has chosen for 'disciplinary institutes' rather than for multi-disciplinary ones. Institutes based on a single scientific discipline traditionally have a great advantage, which the EB appreciates (e.g. all scientists speak the same scientific language), but at the same time they also create a weakness because important developments in science often take place at the borders of disciplines and these may be missed. Also, for achieving the goals of the overall societal driven programmes of LIC multidisciplinary might have been a better option. In the present situation it is, therefore, of great importance for LIC's two clusters to exchange ideas with other different knowledge fields and to further initiate joint actions. In this connection the EB strongly supports the plans of LIC and Leiden University Medical Centre (LUMC) to restructure their interactions and make their collaborations stronger. The same can be said for the interactions between LIC and the Leiden Life Science Park.

Most institutes at universities in The Netherlands have an International Advisory Board (IAB). LIC has one as well, but it does not seem to be very active according to the Self-evaluation report and the discussions with the director. The EB suggests to reactivate this IAB and have it convene regularly (perhaps every two years) to help establish the strategy of LIC and further define the research themes and other related matters. An IAB consisting of high profile scientists with specific experience in running similar large international institutes will also be helpful in increasing the international visibility of the institute. The latter is very important and should receive more attention from the director and staff. There are also other ways of bringing LIC in a more focal point of attention. LIC may consider to organize annually an institute symposium, where internationally renowned scientists explain new developments in the fields of the two clusters and where Ph.D. students and post-docs give presentations for an international audience. LIC may also wish to bring important international conferences to Leiden, more than it does now. The Chemical Biology cluster is linked to a Dutch Gravity programme, which increases its visibility. The EB hopes that the Energy & Sustainability cluster will also manage to be connected to such a program in the near future.

LIC has hired a relatively large number of excellent young scientist in recent years, mainly due to the extra finances coming from the Sector plan programme of the Dutch government. This hiring

has given new and important impulses to the research activities with as a result that LIC is now better prepared for the future. According to Chart 1 in Appendix 4 the ages of the scientific staff are well in balance. The tenure track system seems to work adequately and the criteria for tenure are sufficiently clear for those involved. Unfortunately, as reported by the Director, in the future fewer tenure trackers can be hired and new positions will be created mainly when Professors are leaving or retiring. The EB wonders how many tenure trackers eventually can be appointed to full professor. Are there any regulations (financial or otherwise) restricting the number of full professors and if so how are these handled?

The infrastructure of LIC including the new labs is excellent. The EB is also very pleased with the new cell observatory, which is a bottom-up initiative that will enhance the collaborations of the Chemical Biology cluster with other departments and institutes in Leiden, e.g. LACD, IBL, and LION. For the future it is important to keep an eye on the availability of indispensable instrumentation, e.g. NMR. Early applications to the Permanent Committee for Large-Scale Scientific Infrastructure of NWO together with NMR groups from other universities (Utrecht, Nijmegen, Wageningen, and Eindhoven) will be needed.

***Based on the received documentation and the discussions with director and staff the EB has obtained a good impression of the viability of LIC. Taking everything into account the EB rates this aspect as 2 (very well equipped for the future).***

## 2.4. PhD programme

At the end of the first day of the site visit the EB had the opportunity to have discussions with representatives of the Ph.D. students, which were extensive and very pleasant. The students felt that the Ph.D. programme and their training were well structured and overall they were quite happy with the working conditions and the quality of supervision. The EB notes that the current strong increase in Ph.D. student numbers is very positive, but may cause problems because not enough staff for coaching and mentoring may be available in the coming years.

The EB learned that there are four transferable skill courses for Ph.D. students, which are mandatory, but many students had mixed feelings about their added value. For instance, the Academic writing classes seem to be focussed on grammar and not on the story telling aspect that writing a paper requires; an additional higher level course could be usefully added for fluent English users. All students participate in the programmes of National Graduate schools, the most important ones being HRMS, NIOK, NMARRS, and NRSCB. Voluntary courses can be chosen from the lecture programmes of these schools. Students have the possibility to go to international conferences, but the frequencies by which this happened differed from student to student. There seems to be a travel budget for them, but this budget is not transparent and varies from group to group. The EB recommends to re-examine the training courses and the possibilities for travelling and conference visits for the students.

The selection of the Ph.D. students, who in most cases are paid from individual grants of the PI's, follows a standard protocol, in which also the scientific director plays a role to guarantee that the best candidates are selected. This is a good way of operating, although it is not clear to the EB whether indeed the best students are chosen and whether in general LIC is capable of attracting top students. This has also to do with the already mentioned visibility of the institute (see section 2.3 of this report). The Dean of the Faculty formally appoints the supervisor and since 2015 also a second supervisor. The student writes a research and a training plan, which is evaluated after nine months in the form of a progress report and a meeting with the director and supervisor. If the report is approved the student is allowed to continue and receives a contract for the rest of the Ph.D. period. The students commented that after this initial meeting in nearly



all cases no follow up meetings were organized. Many of them felt very uncertain about the progress of their work and whether they would be able to finish within the fixed four years. The EB feels that LIC should consider to appoint for each Ph.D. student an independent thesis committee that monitors the progress of the work through in-depth meetings with each student on a yearly basis, and advises the supervisor when the student should stop with experimental work and start writing.

Unfortunately, only 3% of the students successfully defends the thesis after four years, but this number increases rapidly after five years to 65%. A total of ca. 12 % never finishes his or her Ph.D. thesis. According to the director this relatively high drop-out number is the result of the fact that several PI's left LIC, while taking their students with them. These duration and success rate numbers are probably not very different from those of other universities, although the percentage of students that stop at LIC is still relatively high. The EB strongly feels that the thesis work including writing should be finished within four years. A further improved selection process and a still better supervision (including motivation) of the student may be needed to increase the percentage in-time finished theses. In order to reduce the length of the Ph.D. programme some other universities offer bonuses of varying height if the student finishes within certain periods. A similar procedure seems to be in place at LIC, but apparently it does not work as well as it might.

Ph. D. students have an obligation to teach as part of their training programme, very often involving the supervision of practical courses by them. From the discussions with the students it became clear that they were unhappy with the current procedures of assigning teaching tasks and that the teaching loads in general were too heavy. The director and educational board may wish to look into this and give this issue a follow-up. Since extensions are currently provided to students on the basis of teaching contribution, an alternative approach would be to reallocate these funds to appoint dedicated teaching staff, with a lighter touch teaching role for PhD students to enable them to gain relevant experience without the current high burden.

After having finished their Ph.D. work most of the students easily find a first job, which is excellent, and for ca. 70% this is in research. It is not clear from the Self-evaluation report whether the supervisor and co-supervisor help students in finding their first positions. According to the interviewed students more mentoring towards the period after Ph.D. would be welcomed. An obligatory exit interview as part of the Ph.D programme procedure, therefore, is highly desirable.

Thesis work should lead to papers in scientific journals. It is not clear from the Self-evaluation report if explicit requirements have been set by the Faculty of Science and LIC for the number of papers (corresponding to publishable thesis chapters) that should be produced as part of the Ph.D. work. A further question is how many theses have received the label cum laude in the period of the assessment and whether this number is similar to the numbers of other institutes in Leiden and of other universities.

## **2.5. Research integrity**

The academic integrity practice of LIC follows the Netherlands Code of Conduct for Scientific Practice of the VNSU and the university has appointed a confidential advisor on academic integrity. In the past period two cases of suspected violation of academic integrity were reported and these were handled adequately. The special mandatory course on scientific integrity for Ph.D. students introduced by the director is welcomed. Also the separate check of the Ph.D. theses with respect to scientific integrity is laudable.

Th EB noted that special regulations have been established with regard to the management and

storing of research data, which is very positive. LIC might consider to set up a special, centralized depository bank in line with what other universities are currently doing.

Altogether the EB concludes that the safeguarding procedures for research integrity are in place and appear sound.

## **2.6. Diversity**

The gender issue at LIC is problematic: less than 10% of the full professors are female (see also section 1.4.1 of this report) and the percentage of female associate professors decreased in the period of the assessment from slightly below 30% to ca. 15%, which is worrying. Further actions are clearly needed, although it is also known that in general high-profile female professors and other female staff are difficult to hire. Fortunately, the number of female postdoctoral students is increasing, as is the number of female tenure track staff members (Charts 2 and 4, Appendix 4). A general strategy should be developed and a coordinated action with other institutes of the Faculty of Science taken, involving, among others, special training, coaching, and career programmes for women, to solve this difficult problem. One might also consider to put the tenure track system for male candidates on hold for some time in order to favour the hiring of female staff. On the other hand the EB noted in discussions that not every woman would be happy with such a move, because she would like to be judged and hired on her own merits in competition with male candidates. LIC has indicated that the gender issue is a high priority of the institute for the coming years and the EB is content with this statement and looks forward to further actions. Consideration could be given to the 'Athena SWAN' model which has strongly impacted codes of practise in the UK by awarding nationwide rankings to Universities on the basis of improving equal treatment of staff. Further pressure should be brought to bear on the national administrators of the current tenure system to implement with immediate effect a firmly-enforced and well-publicised extension of the maximum permitted tenure period (termed 'stopping the clock' in comparable tenure systems) for staff gaining substantial responsibilities as primary carer (particularly new mothers) during tenure track.

The balance between experienced and young staff members at LIC is adequate as already mentioned in section 2.3 and does not require special attention. No information is available about the number of foreign scientists and scientists from ethnic minority groups (in Dutch 'allochtonen') working at LIC, but special actions do not seem to be needed here.

### **3. Recommendations**

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The EB recommends the following:

#### **Research quality**

(1) Formally appoint thrust leaders to each of the two research clusters, who also become members of the Management Board.

#### **Relevance to society**

- (2) Further define the societal ambitions of the two research clusters
- (3) Define valorisation indicators
- (4) Increase the funding from contract research to well above the current 10%
- (5) Increase spinoff and patent licensing activities
- (6) Focus outreach activities more on teachers than on high school students

#### **Viability**

- (7) Better define what a research group is
- (8) Define an overarching research theme for the cluster Chemical Biology
- (9) Consider expanding the cluster Energy & Sustainability
- (10) Define the position and role of bridging groups between the two clusters
- (11) Revitalize the International Advisory Board
- (12) Increase the interactions with LUMC and the Leiden Life Science Park
- (13) Increase the international visibility of LIC
- (14) Take action to ensure the availability of indispensable instrumentation (e.g. NMR)

#### **Ph.D. programme**

- (15) Reduce the average duration of the Ph.D. programme
- (16) Appoint an independent thesis committee that monitors the progress and success of the Ph.D. work annually
- (17) Create sufficient coaching staff for the increasing numbers of Ph.D. students
- (18) Introduce exit interviews for Ph.D. students

#### **Research integrity**

- (19) Create a LIC depository bank for research data

#### **Diversity**

- (20) Take firm steps to enhance the gender balance in LIC

## **LIC's research groups**

## 1. Introduction

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As mentioned earlier in this report, LIC has restructured itself around two major research areas: Chemical Biology and Energy & Sustainability. The LIC Chemical Biology research is conducted by seven research groups: the Bioorganic Synthesis (BIOSYN) group, the Macromolecular Biochemistry (MACBIO) group, the Metals in Catalysis, Biomimetics and Inorganic Chemistry (MCBIM) group (this group participates in both research areas), the Supramolecular and Biomaterials Chemistry (SBC) group, the Medical Biochemistry (MBIOC) group, the Biophysical Structural Chemistry (BSC) group, and the recently created Molecular Physiology (MOLPHYS) group. The LIC Energy & Sustainability research is conducted by four research groups, namely the Theoretical Chemistry (THEOR) group, the Metals in Catalysis, Biomimetics and Inorganic Chemistry (MCBIM) group (which also participates in the other focal area), the Biophysical Organic Chemistry (BPOC) group and the Catalysis and Surface Chemistry (CASC) group.

In this part of the report, the EB gives its evaluation of the 'research quality', 'societal relevance' and 'viability' of each of the research groups. In some cases, recommendations have been added. The EB first discusses (in alphabetical order) the research groups belonging to the Chemical Biology Cluster. After that, the Energy & Sustainability groups are evaluated. The MCBIM-group will be discussed as part of the Chemical Biology cluster, even though it is part of both clusters.

## **2. Chemical Biology cluster**

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### **2.1. Bioorganic Synthesis (BIOSYN)**

The group consists of four PIs (Prof. Overkleeft, Prof. Van Marel, Dr. Codee, Dr. Van Kasteren), and three associated staff (Dr. Van der Berg, Dr. Filippov, Dr. Florea), with a total of 37 PhD students and 7 postdoctoral staff. The group has particularly strong expertise in the synthesis of complex organic and biological molecules, e.g. carbohydrates, nucleic acids, peptides, and lipids, and uses this expertise to solve important problems in the fields of Chemical Biology and Medicinal Chemistry. Activity-based profiling and related probes are a focus of this group, with glycosidases and the (immuno)proteasome being representative targets in which BIOSYN has led the field internationally.

#### **Research quality**

For a group of four PIs BIOSYN is unusually comprehensive in the set of chemistry it develops and applies, and the quality and particularly the volume of research output generated. BIOSYN's status as a 'linchpin' at LIC is well deserved, and it is a mainstay in terms of major grant income. The grantsmanship of Overkleeft in particular is a major asset to the LIC, with substantial contributions from an ERC Advanced Grant and co-leadership of a Gravity programme in chemical immunology, amongst others. The quality of the group as a whole is excellent and the PI's are world-leading in their field, with strong grant income across the board. Since the last evaluation the problem of productivity has been comprehensively solved; during 2010-2015 the number of papers has increased steadily, amounting to 185 for Overkleeft and 119 for van Marel, for example, and are published in top journals (JACS, Angew. Chem, etc.). Proportionate outputs are being achieved by Codee and Van Kasteren, and the strength and great potential of both these younger tenure trackers is an excellent sign for the future. With this volume has come strong metrics in terms of total citations and h indices. Prof. Overkleeft has received multiple awards, recently including the Jeremy Knowles Award of the RSC (UK), and is a member of the Board of many scientific journals. The tools developed by this group have global reach, and they are the go-to group for biologists working on glycobiology-related chemical tools. The collaborations with Davies (York) and van der Hoorn (Oxford) are good examples, and have led to some high-impact research outputs.

Overall, the research quality of BIOSYN is outstanding and at an international level of excellence. Going forward, the large number of publications and students raises potential challenges of managing the balance between volume and focused targeting of the highest profile journals; this should be carefully considered. The PIs give a good number of plenary and invited lectures at conferences, but still limited in proportion to the volume of published output; this could be strategically expanded to maximize international impact. The next challenges will include increasing impact on biology, and maximising the potential of their chemistry and probes in the field of drug discovery and therapeutics. Clear plans are in place to deliver on these objectives, including in collaboration with other institutes, and strong progress is expected as a result.

#### **Societal Relevance**

The topics studied by the group are highly relevant for society, above all in the fields of biotechnology and healthcare. BIOSYN has been very active in distributing its tools and probes widely to other labs, and this has resulted in a broadening of scientific and societal impact. Multiple patents have been filed, but more support could perhaps be provided by the University to enable these outputs to be converted into spinouts or licensing opportunities. Increasing engagement with industry could be an objective for the future, although this needs to be balanced against the need for students to publish their work and distribute tools as widely as

possible; clearly patenting should only be undertaken when there is a business case to do so. Increasing impact on drug discovery and therapeutics could also be an important goal, and will benefit from increased industry engagement and interactions with the medical centre and through the Gravity programme.

Overall, the contribution to society is very good to outstanding, with the potential to deliver increasing impact in future through closer engagement with medicine and industry.

### **Viability**

The approach to securing internal expertise is very solid, with appointment of Florea and Filippov, and clear plans for the future. A very good development has been the appointment of van der Stelt as leader of an independent group; this was not a trivial transition from industry to academia and then to tenured professor, and BIOSYN leadership should be commended for recognizing potential and enabling it appropriately. The appointment of Van Kasteren is also very positive, and nicely integrated with the chemical immunology initiative. There is outstanding career development of students and postdocs, with good numbers of students and postdocs going on to academic leadership. There is also commendable development and retention of female PhD scientists in this group.

Overall, the viability of the group is excellent. The leadership is consolidated with excellent younger PIs, and has an outstanding figurehead in Overkleeft. The successful implementation of major strategic initiatives (drug discovery hub with LUMC, ICI, etc.) will be very important for future viability.

### **Recommendations**

- Maintain and continue to grow outstanding research profile in chemical biology;
- Explore new opportunities for improved external visibility;
- Formulate explicit strategies to deliver increased impact on fundamental biology and societal/economic impact;
- Deliver on existing plans to invigorate and develop interactions with LUMC and local environment.

## **2.2. Biophysical Structural Chemistry (BSC)**

The Biophysical Structural Chemistry (BSC) group consists of one PI (Lecturer Dr. Pannu), one postdoc, 4 Ph.D. students, and a technician. The research of the group is focused on the development of computational methods that can be applied in structural biology, especially in X-ray crystallography. The group leader initially worked together with Prof. J. Abrahams, who left Leiden University. Since the departure of Abrahams, Dr. Pannu obtained an STW-HTSM grant (2014) and a ZonMW Middelgroot grant (2016). The software developed by the group has been widely employed in many laboratories worldwide. The group is rather small, especially in comparison with other groups at LIC, although perhaps not by comparison with other groups undertaking similar research. The group shows running collaborations with many different LIC groups, including MBIOC, BIOSYN, MCBIM, MOLPHYS, BPOC, and SBC, which are not always underpinned by additional staff or students, leaving the PI with considerable direct responsibilities for running projects.

### **Research quality**

The group leader, Dr. Pannu has published around 50 papers, with a Hirsch-index of 21 (Google Scholar) at the time of evaluation. The h-index of the leader is not especially high for a PhD with 15 years postdoctoral experience, particularly when embedded in a highly collaborative environment like LIC. Pannu has contributed to two software packages (CCP4 and REFMAC5) which have been highly cited due to the fact that they are applied whenever a structure is solved. Taken together with a historical contribution to Crystallography & NMR System (CNS) in 1998, the total citations of these papers amounts to >25000. Pannu took a coauthor role in these papers. In the period 2010-2015, he has published 18 papers, which is not high, certainly when compared to other groups at LIC, and Pannu is corresponding author on only a fraction of these. Aside from the highly cited contributions above, the total number of citations since 2011 amounts to only ca. 130, which is substantially below the LIC average. However recent papers in more prominent journals (e.g. Structure, Nature Commun) suggest that there is the potential for an upward trajectory in the future. Regarding publications in collaboration, output takes place in mid-tier journals. Since structural biology is a highly collaborative field (structural biologists must generally collaborate to have impact) the volume is not considered to be large enough to be highly competitive, particularly when internationally leading groups publish in top tier journals on a regular basis.

The EB detects a lack of substantial wet lab activities outside the collaborative provision of crystallography service, and the group lacks a visionary focus or unifying 'grand challenge' underpinning the majority of their current research work. These points are considered to be a weakness, and a potential barrier to higher quality outputs in the future. According to the information provided and the interview, the current status of the group seems to be more a high-quality service (X-ray structure solution) 'provider' than a group with an independent and transformative research vision.

### **Societal relevance**

From an overall perspective, the development of methodologies for the determination of the structures of proteins and assemblies of proteins that are difficult to crystallize is highly relevant for the scientific community. It is also important for society because the group focuses on structures that may give insight in the mechanism of diseases. Proof for this is the fact that the algorithms (free-software format) previously contributed to by the group are highly cited by colleagues and are frequently applied. The outreach activities are not strong and the interactions with industry are rather limited at present, probably since the policy of the group is to develop



free-software for data analysis. This may change in the future, but is currently a weakness of the group.

### **Viability**

At present and with the current organization, the viability of the group is questionable. Its size is small and the output (aside from historical contributions to globally applied software packages) is modest. However, recent funding successes and the potential for new industry collaborations suggest that the Pannu group could make a valuable contribution to LIC in the future. Nevertheless, with just one PI who is not a full professor, the group remains too small to have international impact.

The EB considers that a better integration with LIC scientists is crucial for the viability of BSC. One possibility for the near future is that the group is merged with another group that has a need for X-ray work. In this context, the MacBio group may be a natural choice, which should be explored. From a scientific perspective the areas where the group is going to work on in the future, as foreseen by the PI, are not ambitious enough, and there is a lack of formulation of big questions or the definition of a grand challenge. All together this may have contributed to a lack of ERC funding and a lack of expansion of the group. Another possibility would be to transform the group and its expertise into a formal X-ray crystallography facility to help LIC scientists with structural biology problems. Alternatively, the group might be more successfully embedded in a bigger crystallography center than present at LIC, where its unique X-ray solution technologies seem to be under-utilized.

### **Recommendations**

- Formulate a strategy to strengthen structural biology at LIC by integration of BSC with another group, or by re-defining BSC as the Institute's facility for protein structure;
- Explore the integration with the MACBIO group, towards the creation of a strong structural biology niche.

## **2.3. Macromolecular Biochemistry (MACBIO)**

The Macromolecular Biochemistry group is composed of three PIs (Prof. Ubbink, Dr. Dame, and Dr. van Ingen) with a total of 16 Ph.D. students, 2 postdocs, and 3 technicians. The group focuses on the structure-function relationship of proteins using NMR, with special emphasis on the application of paramagnetic NMR methods. It has a clear technical strength in the development of new NMR approaches, with the ambition to apply these to very difficult systems. They also employ other biophysical techniques, such as force spectroscopy and fluorescence techniques. More specifically, the dynamic nature of protein structures is probed by these techniques. Recently, Dr. Dame and Dr. van Ingen have brought in new research themes, e.g. the study of the regulation of chromatin function.

### **Research quality**

The use of paramagnetic NMR to study large protein complexes is very original. Indeed, in this field, the group is leading nationally and increasingly internationally. Several papers have been published in top journals, including Science, PNAS, JACS. The international reputation of Prof. Ubbink is excellent and the younger scientists are also showing very good performances. The EB learnt that Dr. van Ingen is leaving to accept a position at Utrecht University (National Facility for NMR), which presents a future challenge for a group that otherwise has a manageable and competitive size (16 PhDs, 2 postdocs).

The group is successful in terms of grant income and the hiring of tenure trackers, international recognition (Human Frontier Science Programme, etc.), and publication output, particularly in collaborative projects. However, there is room for the individual strengthening of the publication output (Dame), and research income (lack of ERC income). Publications in the top tier journals tend not to originate from the group itself but are the result of collaborations.

Internal collaboration is quite effective, with several shared PhD students. Indeed, there has been a very nice interaction with BIOSYN around paramagnetic probes. The renewal of the research focus to include chromatin biology is a success and there is potential for world-leading research in the future. For the coming years, there seems to be an untapped potential to integrate the NMR strengths of the group with modern drug discovery, which could attract major funding. In this context, the plans to target antibiotic resistance are encouraging. In general, stronger industry interactions should be developed where possible.

### **Societal relevance**

The use of paramagnetic NMR methods to study the dynamics of proteins and assemblies of proteins is of high societal and industrial relevance. There are excellent possibilities to link these studies to important medical problems and the research topic of Dr. Dame has an intrinsic societal value at the fundamental level, as well as good outreach potential. However, at present the outreach activities and current industry contributions could be strengthened.

### **Viability**

The group is well anchored in the Chemical Biology cluster and with the new research topics brought in by Dr. Dame and Dr. van Ingen, a dynamic group with a strong research portfolio has been established. The exit of Dr. Van Ingen is a significant concern which should be addressed in the near future, preferably with a tenure track successor. It is advisable that the hired person will be someone with a strong NMR knowledge and an interest in biophysics, and also someone who can be embedded in chemical biology. The reorganization following the previous review appears to have resulted in a strong and viable research grouping with plenty of students. The two

remaining PIs are strong researchers in their own right, and there are no concerns with the general viability and trajectory of the group.

As mentioned above (see the BSC group), a further reorganization is possible by adopting the BSC group to make a new strong structural biology group. A disadvantage is that there is no direct overlap in the research activities of MACBIO and BSC. Nevertheless, both groups are already cooperating, which is helpful. The presence at LIC of Prof. De Groot (BPOC) with his large experience in solid state NMR also opens interesting possibilities for a new strong structural biology niche.

The present infrastructure seems to be very good, with a relatively modern 850 MHz instrument (2013) at hand. The group has also been granted access to the National NMR Facility at Utrecht University, which will be extended in the near future with a 1.2 GHz instrument.

Although the research income of the group seems to be very healthy at the moment, there is still room for further improvement, particularly with regard to ERC grants.

### **Recommendation**

- Foster the creation of a strong structural biology niche, integrating BSC and, probably, BPOC.

## **2.4. Medical Biochemistry (MBIOC)**

The Medical Biochemistry group includes as PIs Prof. Aerts and associated staff member Dr. Boot. Aerts studies lipids and their metabolizing enzymes in relation to health and diseases. Insights into glycosphingolipid metabolism are used to develop therapies for e.g. neurodegenerative diseases. The group started in 2015 at LIC, and before that date Prof. Aerts was affiliated to the Academic Medical Center in Amsterdam (AMC). At LIC Aerts enjoys an environment focused on curiosity-driven research with reduced administrative burdens, although admittedly with less direct interaction with patients. As a biochemist he is a crucial member of the Chemical Biology cluster, with many active collaborations within and outside LIC.

### **Research quality**

Prof. Aerts' group has a manageable size with 9 Ph.Ds and 2 postdocs. They published more than 400 papers, with an h-index 60 and 12000 citations, which is excellent. In the period 2010-2015 the group produced 110 papers, 4 book chapters, and filed 3 patents. The papers are of excellent quality and were published in highly reputed journals. The grant income is excellent with successful funding coming from NWO (TOPPUNT, ChemThem), EU (ERC AdvG/PoC: together with Overkleeft), and industry (Sanofi-Genzyme). Prof. Aerts has received important awards, including the Gaucher Disease Lifetime Achievement Award and the Cle du Lysosome Award. MBIOC performs at an outstanding and internationally competitive level on each metric, i.e. research quality, collaborative aspects, and international profile. In particular, there is a strong and powerful interaction with BIOSYN, which is synergistic for both sides.

### **Societal relevance**

The group is very active in bringing solutions for medical problems as obtained from fundamental biochemical studies to the hospital. The topics are very relevant to society, with strong connections with the Academic Medical Center, where Aerts still has a group. Although this is a niche area, it has very high societal relevance to a small population of patients with an extremely great need. His research programme is a paradigm case of bringing fundamental research to bear on a specific societal problem.

The subject of patents and IP exploitation was discussed at some length with the group. Prof. Aerts has longstanding experience in patenting and explains that it can be a difficult process, with many players that can affect the outcome. A strong level of commitment is required at the institutional level.

### **Viability**

For the next few years the viability of the group is fully ascertained, but planning will be required towards the next review period to deal with the expected retirement of the group leader. With this in mind, the EB feels that the Chemical Biology cluster would benefit from a strengthening of the traditional biochemistry research in the future, particularly around the knowledge field of metabolism and its impact on physiology. This area critically underpins the work of other groups at LIC, and attracting a younger PI to succeed Aerts in this area is something to seriously consider.

Overall, the performance of MBIOC is excellent and internationally leading.

## **Recommendations**

- Continue to play key role in connecting chemistry and biology;
- Give consideration to transition sufficiently far in advance that the right tenured or tenure track scientist(s) can be recruited with some overlap, to ensure no shortfall in physiology expertise.

## **2.5. Metals in Catalysis, Biomimetics and Inorganic Chemistry (MCBIM) (group participates in both clusters)**

The group consists of two PIs (Prof. Bouwman and Dr. Bonnet) with a total of 14 Ph.D. students and 2 technicians. The research of the group focuses on the generation of fundamental knowledge in the field of coordination and organometallic chemistry with applications in various areas including catalysis and bioinorganic chemistry. This variety of applications makes that the group is active in both main research themes of the LIC namely Energy and Sustainability and Chemical Biology. MCBIM is divided in two subgroups, which have some overlap: the first is led by Prof. Bouwman, who works on a large variety of topics, and the second by Dr. Sylvester Bonnet, who mainly focuses on light-induced reactions mediated by transition metal complexes, which have a biologic context.

### **Research quality**

The group has generated a significant number of publications in refereed journals during the period 2010-2015, with a small overlap between the subgroups as reflected by several joint papers and joint PhD theses. Professor Bouwman has published a total of 180 papers of which 41 appeared during the evaluation period. All these were published in peer-reviewed journals, including a very nice *Science* paper in 2010. Dr. Bonnet has published 62 papers, including 36 in the period of this evaluation, which appeared in peer-reviewed journals amongst others in *Angew. Chem. Int. Ed. J.* and in *Am. Chem. Soc.* The group realized 8 PhD theses of which 3 were co-supervised by both PIs.

The EB noticed that the quality of dr. Bonnet's research as well as his visibility among colleagues in the field has increased over the reporting period, which is excellent. Prof. Bouwman's position has remained in a steady state, which is positive, because she has been very active in teaching and the management of education.

The two PI's contribute significantly to the scientific community both locally and at the international level. In particular, Prof. Bouwman serves on the Editorial Boards of Applied Organometallic Chemistry and the European Journal of Inorganic Chemistry (EurJIC). Dr. Bonnet is a member of the Advisory Board of EurJIC and has been elected as a smember of the Young Academy of Europe.

The EB notices that the groups of Prof. Bouwman and Dr. Bonnet are doing important research and have a significant scientific output in their fields. Nevertheless, it feels that the number of topics should be somewhat reduced and that the research should be more focussed.

### **Societal relevance**

The group's research focuses mainly on basic science related to coordination chemistry and particularly to catalysis and bioinorganic chemistry. Most of the research output does not have immediate applications, but is obviously necessary to build up a sufficient body of knowledge so that the technological world can benefit from it. Despite its focus on fundamental problems it is nice to see that the group has filed six patents in the period of the evaluation, which is excellent. In addition, the PIs have made a significant effort on transmitting the science they have generated to the general public, through a number of outreach activities, which is outstanding.

## **Viability**

The group is a respected member of the fundamental coordination chemistry community. Both subgroups have managed to attract significant funding both from governmental institutions and also from private companies. In this connection it is nice to see that Dr. Bonnet has been awarded both a Vidi and an ERC Starting grant, which is a great stimulus for himself and the group as a whole.

MCBIM is active in two research clusters, which requires a clear vision with regard to where to go in the future. It also creates a great responsibility for the PIs because they have to put extra effort in keeping up with what is going on in two rather different research areas. The EB wonders whether this will not create too much pressure and stress in the future and recommends to reconsider this dual position, also because the group has only 2 PIs.

## **Recommendation**

- Reconsider MCBIM's position as being a member of two quite different research clusters. This may require a redefining of the research plans of the group and its research portfolio.

## **2.6. Molecular Physiology (MOLPHYS)**

This new group started in 2016 and was initially incorporated within BIOSYN. The group leader (Dr. van der Stelt) is supported by part-time Prof. Stan van Boeckel, who is a world leading carbohydrate chemist. The group focuses on the design of new drugs and activity-based probes, e.g. for metabolic syndrome and neurodegenerative diseases. Both van der Stelt and van Boeckel have a strong background in industry (Merck-Organon). The group includes 18 PhDs and 4 postdocs and has strong internal collaborations with BIOSYN and is engaged in the Cancer Drug Discovery Initiative (a public-private collaboration).

### **Research quality**

Dr. van der Stelt has published >50 papers to date and filed 6 patents. He has received various grants (ZON MW, Hoffmann-La Roche, Echo, Echo-stip) and is partner in a Gravitation programme. Papers are being published in top journals (Nature Comm., JACS, Angew. Chem.) and have many international authors. Dr. van Stelt is highly visible, for example as the organizer and host of the 2018 meeting of the International Cannabinoid Research Society. His outstanding collaborative network is exemplary and one of the strongest set up by an individual PI at LIC, partly due to his strong industrial background.

MOLPHYS is a new, vital group headed by a very dynamic PI, who gave a highly engaging presentation to the EB. The decision to allow van der Stelt to start an independent group is wise and well-deserved. The EB hopes that he will receive tenure in 2017. The publication output was initially slow for reasons of transition, but is now rising very fast, with a commendable dedication to getting strong science published in the top-tier journals. The EB believes that with further support this group will become one of the strongest at LIC with great potential for high impact mission-oriented research.

Overall the performance is excellent with a great future potential. The EB notes that the group has a very large size for a single PI and although the PI has indicated that he can manage this, partly by having co-supervisors, it feels that there is a need for rapid recruitment of additional staff. Computational drug design and in vivo models are both areas where there could be a strong potential for synergy.

The formation of a group working in the area of modern drug discovery is an excellent development for LIC as a whole. For the future it will be important to ensure that the activity of the group remains focused and is sufficiently supported in order to be successful in a highly competitive area, where comparable international groups (e.g. in Germany, UK, and USA) have more extensive infrastructure available. The EB was happy to see that the PI has clear plans to focus on specific therapeutic areas and fully appreciates the need for the involvement of biology in this type of research and the presence of a dedicated local infrastructure.

### **Societal Relevance**

The topic of the research (drug design) is highly relevant for society. The group is strongly involved in networks with institutes worldwide. The connections with industry (Hoffmann La Roche, Lead Pharma, Acerta Pharma, NTRC) are excellent, with a strong focus on applications (6 patents). The relevance to drug discovery and disease is obvious, and the group has a strong outreach to the scientific community through the organization of meetings, etc, and to society more widely through media coverage. It is also one of the stronger groups at LIC in terms of industry interactions. Overall, the contribution to society is outstanding.



## **Viability**

Van der Stelt has made a great start with his new group. The next objectives will doubtless include securing further programmatic funding (ERC etc.), further support from LIC in terms of staff, and support to exploit IP outputs. The current target/disease space is certainly highly viable, and the PI is fully aware of the competitive landscape, whereby currently promising targets may be invalidated by outside parties. The EB notes that endocannabinoids are a new area for LIC and that this needs careful integration for maximum benefit.

Overall, the viability is excellent with a strong leadership and a great future potential.

## **Recommendations**

- Nurture this new group's momentum and support it with sufficient resources and staff to ensure future success with maximum societal impact;
- Carefully monitor supervision load on PI to avoid 'burn out'.

## 2.7. Supramolecular and Biomaterials Chemistry (SBC)

The group is composed of Prof. Alexander Kros (group leader), Dr. Kieltyka, and Dr. Schneider. Dr. Blokhuis and Dr. Oltshoorn are associated staff members.

The research of the group is situated at the interface of supramolecular chemistry and biomaterials science and is aimed at studying transport phenomena in a range of *in vitro* and *in vivo* systems. The goal is to acquire knowledge that can be used in the future to e.g. develop sophisticated diagnostic tools, to better understand genome/proteome relationships in diseases, and to elaborate procedures for the production of induced pluripotent stem cells for regenerative medicine. Topics include membrane fusion in well-defined model systems, the design of new biomaterials (e.g. based on squaramides) for cell programming, biosensors, biomolecular transport, and DNA sequencing through porous 2D membranes. The work involves molecular and macromolecular synthesis, imaging studies, studies on biomembranes, hydrogels, cell differentiation studies, and modification of graphene layers. The staff members collaborate with specialists from (bio)physics, biology, and medicine.

### Research quality

After the departure of the previous group leader and chair holder (Prof. Fraaije) the focus of the research was changed considerably and for the better. The group has made a swift start in a new and challenging research direction. The quality of the work is excellent as can be concluded from the fact that the papers have been published in top journals, e.g. Nature Commun., JACS, Angew. Chem., ACS Nano, Chem. Science, and Advanced Materials. The number of papers is considerable (ca. 80 in the assessment period) and the citations are high (estimated roughly 3000 citations), certainly when taking into account that this is a very young group.

Prof. Kros was the first staff member at the LIC to receive an ERC grant (ERC starting grant) in 2009 and since then the group has secured more funding in the form of another ERC starting grant, two ERC proof of concept grants, a prestigious VICI grant, a VIDI grant, and four VENI grants, which is excellent.

The group has an extensive network of collaborations, both within The Netherlands and outside. Prof. Kros is an editorial board member of the journal Scientific Reports (from the publishers of Nature) and acts as reviewer of the journal Chemical Biology. He has been a co-chair of international conferences and is a frequently asked speaker at universities and at international meetings (> 50 invited presentations since 2010).

Altogether the group scores very high and is making contributions at an international level.

### Societal relevance

The chemistry of biomaterials, drug delivery, biosensors, and membrane fusion is highly relevant for society and industry. The group has an open eye for applications and the connections with industry are very good, given the substantial financial support that has been received (e.g. from Hal Allergy Group, CrossBetaSciences, Declathon). Also the number of filed patents (7) in the past period confirm this strong link and the high societal impact.

The conclusion is that the contribution to society is outstanding.

### **Viability**

This is a young and dynamic team with good ideas and the potential to transform these ideas into products that are useful for society. The hiring of the new tenure track staff members is a very positive move and has brought in new research lines. The group fits well within the cluster Chemical Biology of LIC and is expected to grow further in strength and size with the expectation that it will become in the future one of the top research groups in The Netherlands and worldwide. The EB appreciates the high commitment of the group and its eagerness to do top class research. On the other hand it has some concern about the large number of topics the group is working on and the broadness of the projects, ranging from cell programming to graphene. Also the rapid growth of the group (from zero to over 30 Ph.D. students and postdocs) might lead to coaching problems.

Altogether the EB feels that the group is very well on its way and has excellent prospects for the future.

### **Recommendation**

- Limit the number of topics and monitor the broadness of projects.

### **3. Energy & Sustainability cluster**

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#### **3.1. Biophysical Organic Chemistry (BPOC)**

The group studies the mechanism of photosynthesis and develops low molecular weight artificial photosynthetic systems. NMR techniques, electron microscopy, and theoretical calculations are used as tools to achieve the research goals. The group has a strong reputation in NMR spectrometry applied to large natural molecules. The group leader Prof. de Groot is a well-recognized and visible scientist in the field of biophysics and especially in the use of NMR as a tool for characterization of complex natural systems. Dr. Pandit (tenure track Assistant Prof.) has been recently incorporated in the group (2013) and comes from the group of Prof. Rienk van Grondelle, a world leading group in energy transfer and trapping in photosynthesis. The group also contains three lecturers ('docenten'), all of which are active in research. Associate Prof. Buda provides theoretical support, in particular with respect to DFT calculations. The group has 11 PhD students.

#### **Research quality**

The group is doing very nice research and has been very active during the period 2010-2015, resulting in a significant output of papers of which some are joint efforts of the group members. Prof. de Groot has published a total of 210 papers (43 during the period of the evaluation) in peer reviewed journals, which are citing very well. Dr. Pandit's research output before 2015 comes mainly from her previous affiliation, as she was only incorporated into the group in 2013. She has published 22 papers overall, 13 of which were within the period 2010-2105.

Dr. De Groot's is a recognized scientist in his field who formulates important and challenging questions, which he addresses successfully in a very creative way. His scientific output is of high quality. He has supervised 9 PhD theses, which were successfully defended during the 2010-2015 period and he has been invited to lecture at different scientific congresses and meetings. He has also filed four patents during this period, which shows that he has an open eye for applications and the transfer of fundamental knowledge to society.

#### **Societal relevance**

The research of the group is devoted mainly to basic science, trying to understand and characterize phenomena that occur during photosynthesis and related processes. As such the work does not have immediate applications in the technological world, but it is obviously of paramount importance for the understanding of nature's way of functioning. The work fits very well within the Dutch Science Agenda and is very important for society. Despite the fundamental focus the group has filed four patents in related topics (see above). In addition, Prof. de Groot has done a significant effort in communicating their work to the general public through a number of outreach activities.

#### **Viability**

The group is highly respected in the field of NMR applied to large natural molecules and is one of the key players in this field. Prof. de Groot has been awarded a number of public grants from FES, NTWO and others; hence his future research plans seem secured. In addition, Dr. Pandit was awarded with a Vidi grant in 2013, which further strengthens the midterm financial goals of the group, also giving scientific credit and visibility. However, for the mid- to long-term the group should consider a further expansion at the PI level (in addition to Dr. Pandit), e.g. via the incorporation of an additional junior professor, which would guarantee a successful transition after Professor de Groot's retirement.

## **Recommendations**

- Consider incorporating a new staff member to ensure that the knowledge acquired by the lab is not lost and can be further exploited in the future;
- Consider starting new projects with colleagues in the Biological Chemistry to further strengthen the group's position both within the LIC and in the international arena. In this context, the possibilities of creating a strong structural biology niche, including MACBIO and BSC, could be explored.

## **3.2. Catalysis and Surface Chemistry (CASC)**

The research of the group focuses on the identification of surface-catalyzed chemical processes that are relevant for the sustainable production and storage of energy into fuels and chemicals. The group consists of one full professor (Prof. Dr. Koper), one assistant professor (Dr. Juurlink), two tenure track assistant professors (Dr. Groot, Dr. Hetterscheid) and associated staff (Dr. Fu). A particularly strong point of the group is the combination of electrochemical experiments at the electrode/electrolyte interface (Koper) with related studies at the surface/vacuum interface (Juurlink). The appointment of Dr. Groot with her focus on heterogeneously catalyzed reactions at the solid/gas interface has definitely strengthened the scope of the group, as has Dr. Hetterscheid's work on surface-immobilized metal-organic electrocatalysts for water splitting, which also serves as a link to the other, more molecularly oriented groups in the Energy & Sustainability cluster. The experimental studies are nicely combined with calculations, mainly based on quantum chemical approaches, but largely related to electrochemical systems. The combination of the PI's in the group allows them to maintain and strengthen their own independent research profile and at the same time work closely together.

### **Research quality**

The group is one of the top groups in its field worldwide. It has been very productive in the period from 2010 to 2015, as far as refereed research articles are concerned. More than 150 articles were published, 127 of them (co-)authored by Prof. Koper, of which a significant number appeared in high-profile journals such as Nature Comm., Nature Chem., J. Am. Chem. Soc., Angew. Chem., Chem. Soc. Rev., and ACS Catalysis. The strong cooperations within the group is reflected by several joint publications. Prof. Koper certainly stands out with in total more than 10,500 citations and an H-index of 58 according to the Web of Science, but also the work of Dr. Juurlink, Dr. Groot and Dr. Hetterscheid is well-recognized by the scientific community, given the present status of their scientific careers.

Prof. Koper is very visible, which is reflected by more than 100 invited presentations at universities and international conferences since 2010. He received several awards (e.g. Carl Wagner Memorial Award, Helmut Fischer Medal of DECHEMA, JPF Fellow). He is a member of the board of various journals and is Associate Editor of Catalysis Today and also Associate editor of the most important journal in the field of catalysis, i.e. the Journal of Catalysis. The group is capable of raising substantial funding for its research activities (e.g. NWO Top grant, ERC Starting grant, Veni grant). In sum, the research quality of the group is excellent.

### **Societal relevance**

The research of the group on chemical aspects of energy and sustainability is of the uttermost relevance to society, in order to meet the increasing demand for energy in a sustainable and environmentally-friendly way. As the research of this group focuses on fundamental aspects of atomic-scale processes in (electro-)chemical energy conversion, the insights gained by the research efforts will not be immediately transferable to industry but without such a fundamental approach no long-term progress is possible. Still, there are three patents that have been filed by the PI's of the group since 2010, and there are strong industry collaborations with a number of companies. Furthermore, Dr. Groot and Dr. Juurlink have each written two publications aimed at the general public. Thus the research group makes an excellent contribution to society.

### **Viability**

The group is performing outstandingly and is very well-positioned in the field of fundamental research on surface and interface processes for the sustainable production and storage of energy

into fuels and added-value chemicals. It is vital and has very good ideas with respect to where to go in the future. The younger staff members are eager to make a contribution and have a great potential. The group intends to extend its collaborations, in particular with the Delft University of Technology, which is excellent. This will be very beneficial for the group as it will allow to transfer the insights from the fundamental research in Leiden to the more applied groups in Engineering at Delft. The only comment the EB has is that the cluster in which CASC participates is rather small. In order to make a substantial impact the cluster Energy & Sustainability should be expanded with other groups. Alternatively, the group should seek stronger interactions with groups at other institutes in Leiden (LION?) or at other universities, e.g. Delft (see recommendation in general part of this report).

### **Recommendations**

- Take the lead in the Energy and Sustainability cluster to create a more focused research portfolio of the cluster;
- Expand the theoretical support for the experimental studies related to heterogeneous catalysis.

### 3.4. Theoretical Chemistry (THEOR)

The Theoretical Chemistry group has a clear research profile focusing on the reliable theoretical determination of simple reactions of molecules on surfaces. The first objective is to obtain mechanistic insight at the atomic-level in elementary steps of model chemical reactions that are part of surface-catalyzed processes. The second objective is to provide benchmarks for the reliability of first-principle-total-energy calculations by comparing computed state-resolved reaction probabilities with experimental data. The group develops a database with chemically accurate reaction barriers for molecules reacting on metals.

Recently, the group has also started to use *ab initio* molecular dynamics simulations, which is a more versatile tool, but these simulations are still computationally rather expensive. Through the appointment of Dr. Meyer in 2014 a further research topic in gas-surface dynamics, i.e. the energy exchange of the reacting molecules with the surface, was added to the group, which broadened its scope. Furthermore, Dr. Meyer also brought his expertise in first-principles electronic structure calculations to Leiden. There is a very good synergy between the two PIs in THEOR, in the sense that new methods developed by Meyer are applied by Kroes.

THEOR consists of one full professor (Prof. Kroes), one assistant professor (Dr. Meyer), and one lecturer (Dr. Somers). Prof. Kroes is internationally very well-known for his high-dimensional quantum dynamical studies on the interaction of hydrogen with metal surfaces. The group is very visible within and appreciated by the Theoretical Chemistry community. There are many links with other research groups worldwide.

#### **Research quality**

There are 46 peer reviewed articles co-authored by Prof. Kroes in the period from 2010 to 2015, some of which appeared in high profile journals like PNAS, PRL, and J.Phys.Chem.Lett. The recognition of the work of Prof. Kroes by the scientific community is reflected by in total 6600 citations and a respectable h-index of 42. Dr. Meyer is still at an earlier stage of his career with 25 publications and a h-index of 11.

Prof. Kroes has been very successful in acquiring research grants. The ERC Advanced Grant from 2013 certainly stands out, but there are also prestigious NWO grants. Dr. Meyer obtained a NWO-CW Vidi grant in 2015. The calculations performed in the group are numerically very demanding, but the group has an excellent computational infrastructure. Additional computer time is provided through grants allowing access to national computing centers.

#### **Societal relevance**

The subject of the research, i.e., the interaction dynamics of molecules with surfaces, corresponds to the first and often crucial step in heterogeneous catalysis. It is therefore highly relevant for industry and society, although the scope of the research is on fundamental aspects of this interaction. Prof. Kroes also authored and edited publications aimed at the general public, emphasizing the importance of fundamental research for society and economy.

#### **Viability**

The group will further develop its theoretical and numerical tools to describe the interaction dynamics of molecules with surfaces in a very competitive area, in particular the area of electronic non-adiabatic processes in the interactions of molecules with surfaces. Although there is some overlap in the research interests with the Catalysis and Surface Chemistry group, the interaction with other groups in the Energy & Sustainability cluster is minor and should be



intensified in order to make the coherence of the overall research stronger. The Theoretical Chemistry group certainly has the potential and resources to do this.

**Recommendation**

- Broaden the scope and seek more collaborations within the Energy & Sustainability cluster.

## **Appendices**

## 1. Appendix 1: Curricula vitae of the EB members

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**Roeland J.M. Nolte (Chair)** is Emeritus Professor of Organic Chemistry at Radboud University, Nijmegen, The Netherlands and former Director of the Institute for Molecules and Materials of this university. He is a member of several learned societies, including the Royal Netherlands Academy of Arts and Sciences, the Royal Belgian Academy for Science and the Arts, and the Academia Europaea. He currently holds a special University Chair in Molecular Nanotechnology at Radboud University. His contributions to science have been recognized with numerous award lectureships and several national and international prizes including the Izatt-Christensen Award for Excellence in Macrocyclic Chemistry, the first Royal Netherlands Academy of Science Chair in Chemistry, an Honorary Fellowship of the Royal Netherlands Chemical Society, and a knighthood in 2003. He has served on the editorial boards of many scientific journals, including the journal *Science* (Washington) and the RSC journal *Chemical Communications* (as Chairman).

**Axel Groß** is the Director of the Institute of Theoretical Chemistry at Ulm University, Germany. He studied physics at the University of Göttingen and the University of California at Santa Barbara and obtained his PhD at the Technical University of Munich. After five years as a staff scientist at the Fritz-Haber-Institute of the Max-Planck-Society in Berlin he became Associate Professor of Theoretical Physics at the Technical University of Ulm before moving as a Full Professor to Ulm University. He was the Spokesperson of the Research Unit “Elementary Reaction Steps in Electrocatalysis: Theory meets Experiment” funded by the German Science Foundation. He also served as a Dean of the Faculty of Natural Sciences and as Vice-President for Research of Ulm University, and as the Spokesperson of the Surface Physics section of the German Physical Society. He was the member of several scientific advisory boards. At the moment he is an elected member of the Chemistry Review Board of the German Science Foundation.

**Jesús Jiménez-Barbero** is Ikerbasque Research Professor and Scientific Director at the Centre for Cooperative Research in Biosciences (CIC bioGUNE), Bilbao, Spain. Previously, he was Head of the Department of Chemical and Physical Biology at the Center for Biological Research of the National Research Council (CSIC) of Spain at Madrid. He is the President of the Royal Society of Chemistry of Spain and Manager of the Chemistry panel of the State Plan of Research of the Ministry of Economy and Competitiveness of Spain. He has received different award lectureships and national and international prizes, including the International Whistler Award in Carbohydrate Chemistry. He is ChemPubSoc fellow and serves in the editorial board of many scientific Journals, including *Chemistry European Journal* and *ChemBioChem* (Wiley VCH-ChemPubSoc Europe) and *ACS Chemical Biology* and *ACS Omega* (American Chemical Society).

**Antoni Llobet** obtained his PhD at the *Universitat Autònoma de Barcelona* (UAB) in July 1985, and then moved to the University of North Carolina at Chapel Hill for a postdoctoral stay with Prof. Thomas J. Meyer, until the end of 1987. After again a short period at UAB and at the University of Sussex-Dow Corning (UK) he became a Scientific Officer for the Commission of the European Communities, based in Brussels, Belgium (1990-1991). Then he was appointed Senior Research Associate at Texas A&M University in College Station (USA) from 1992-1993. From 1993-2004 he joined the Faculty of the *Universitat de Girona* where he was promoted to Full Professor in 2000. At the end of 2004 he joined the Faculty of UAB also as a Full Professor. In September 2006, he was appointed as Group Leader at the Institute of Chemical Research of Catalonia (ICIQ) in Tarragona. In 2000 he received the Distinction Award from *Generalitat de Catalunya* for Young Scientists. In 2011 he was awarded the Bruker Prize in Inorganic Chemistry from the Spanish Royal Society of Chemistry (RSEQ) and in 2012 he was awarded with the “Hermanos Elhuyar-Hans Goldschmidt” lecture jointly by RSEQ and the German Chemical Society (GDCh). At present he is a member of the Editorial Advisory Board of “Catalysis Science and Technology” from the Royal Society of Chemistry, “Inorganic Chemistry” from the American Chemical Society, and “European Journal of Inorganic Chemistry” from Wiley-VCH.

**Ed Tate** obtained his PhD in organic chemistry and methodology at the University of Cambridge in the group of Prof Steve Ley, after which he worked at the Ecole Polytechnique (Paris) and the Pasteur Institute (Paris). He took up an independent BBSRC David Phillips Research Fellowship at Imperial College in 2006, was promoted to Senior Lecturer (2010) and then Reader (2012), and since 2014 he has held the Chair in Chemical Biology in the Department of Chemistry, and since 2017 leads a Satellite Group at the Francis Crick Institute. He is a Fellow of both the Royal Society of Chemistry (FRSC) and the Royal Society of Biology (FRSB). He sits on the editorial advisory boards of Cell Chemical Biology, Molecular BioSystems, the Journal of Chemical Biology and the Biochemical Journal, sits on the steering committee of the EU COST action ChemProbes, the committee of the RSC Bioorganic Group, and the ICR/Imperial Cancer Research Centre of Excellence board. He was awarded the 2012 Wain Medal Lecture and Prize and the 2013 RSC/MedImmune Protein and Peptide Science Award in recognition of his research in chemical biology, and was elected FRSC in 2013, and FRSB in 2014. He also received the 2013 President's Award for Excellence in Research Supervision, the 2014 RSC Norman Heatley Award in Chemical Biology, and the 2015 CRUK Programme Foundation Award.

## Appendix 2: Explanation of the SEP criteria and categories

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Extended description of the 4-point scale for categorizing the quality along three criteria

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

## Appendix 3: Programme of the site visit

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### Day 1: Monday 13 February (Golden Tulip Hotel)

15.00-16.00	Preparatory meeting Chair Committee and Secretary
16.00-17.00	Welcome to Committee
17.00-20.00	Preparatory meeting Committee
20.00	Dinner

### Day 2: Tuesday 14 February (room EM1.19)

08.30-09.30	Interview session with Management
09.30-10.15	Interview session Bio-organic Synthesis
10.15-10.30	Break + review
10.30-11.15	Interview session Molecular Physiology
11.15-12.00	Interview session Macromolecular Biochemistry
12.00-13.00	Lunch + review (new Van Arkel room)
13.00-13.45	Interview session Biophysical Structural Chemistry
13.45-14.30	Interview session Medical Biochemistry
14.30-14.45	Break + review
14.45-15.30	Interview session Supramolecular and Biomaterials Chemistry
15.30-15.50	Interview with Head of Education Affairs/Graduate School and Scientific Director
15.50-16.30	Interview with PhD-students
16.30-17.30	Review, writing, preparation
19.00	Dinner

### Day 3: Wednesday 15 February (room EM1.21)

08.30-09.15	Interview session Catalysis and Surface Chemistry
09.15-10.00	Interview session Metals in Catalysis, Biomimetics and Inorganic Materials
10.00-10.15	Break + review
10.15-11.00	Interview session Biophysical Organic Chemistry
11.00-11.45	Interview with Dean
11.45-12.30	Tour of facilities (with possibility to talk to technical staff)
12.30-13.30	Lunch + review (new Van Arkel room)
13.30-14.15	Interview session Theoretical Chemistry
14.15-14.45	Preparation final interview
14.45-15.30	Final interview with management
15.30-17.30	Internal meeting: review, writing and preparation preliminary findings
17.30-18.00	Presentation of preliminary findings (Room GM4.13)
18.00-19.00	Drinks
20.00	Dinner for remaining committee members

## Appendix 4: Quantitative data

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### 1. Composition of LIC staff

Table 1: Composition of LIC staff (2010-2015)

	2010		2011		2012		2013		2014		2015	
	#	FTE	#	FTE	#	FTE	#	FTE	#	FTE	#	FTE
Scientific staff	39	36.4	41	36.7	42	35.5	44	37.1	46	38.7	47	41.1
Post-docs	45	31.4	41	26.9	41	26.3	40	21.3	45	30.0	47	34.2
PhD students*	89	74.7	100	78.1	109	81.4	115	85.2	125	97.2	159	123.7
<b>Subtotal research</b>	<b>173</b>	<b>142.5</b>	<b>182</b>	<b>141.6</b>	<b>192</b>	<b>143.2</b>	<b>199</b>	<b>143.6</b>	<b>216</b>	<b>165.8</b>	<b>253</b>	<b>199.0</b>
Technical support	33	26.1	28	24.3	27	22.3	26	23.0	27	21.8	29	23.9
Other support	17	10.8	15	10.1	15	9.8	16	10.1	17	11.3	15	11.3
<b>Subtotal support</b>	<b>50</b>	<b>36.9</b>	<b>43</b>	<b>34.4</b>	<b>42</b>	<b>32.1</b>	<b>42</b>	<b>33.1</b>	<b>44</b>	<b>33.1</b>	<b>44</b>	<b>35.2</b>
<b>Total staff</b>	<b>223</b>	<b>179.4</b>	<b>225</b>	<b>176.0</b>	<b>234</b>	<b>175.3</b>	<b>241</b>	<b>176.7</b>	<b>260</b>	<b>198.9</b>	<b>297</b>	<b>234.2</b>

The category scientific staff includes tenured and non-tenured staff at the level of full professor (hoogleraar), associate professor (universitair hoofddocent), assistant professor (universitair docent) and senior researcher (onderzoeker).

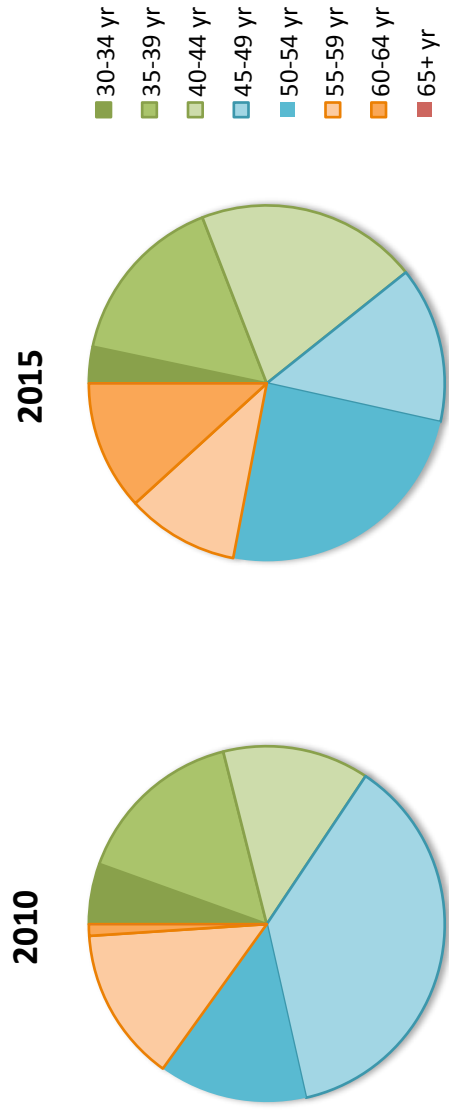
Post-docs include those employed by Leiden University as well as those employed by FOM.

PhD students include those employed by Leiden University and FOM, as well as contract PhDs (externally funded but not employed).

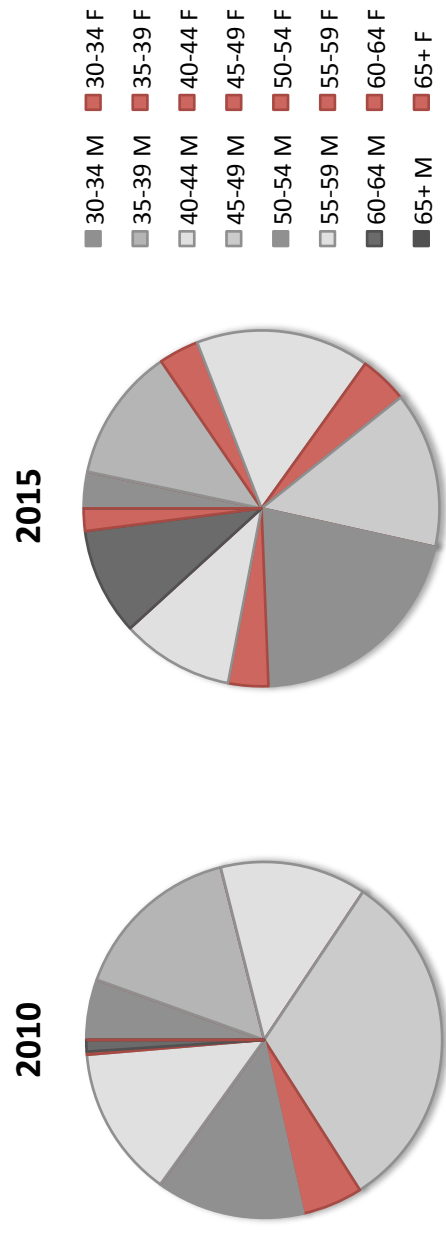
Technical support includes technicians and laboratory assistants working in the various research groups and facilities (NMR, tissue culture), education personnel (studycoordinators), and the central laboratory service (CLD) - personnel involved in preparing the practical courses for several studies. CLD personnel (5 fte in 2015) is officially employed at the LIC, other institutes (mainly LACDR) reimburse the LIC for CLD activities carried out for their fields of disciplines.

Other support staff includes managerial, education (study-advisors) and secretarial personnel.

*Chart 1: Age distribution of the LIC scientific staff*



*Chart 2: Gender-age distribution of the LIC scientific staff*





## 2. Funding

Table 2: Funding based on annual expenditure figures

Funding:	2010		2011		2012		2013		2014		2015	
	FTE	%	FTE	%	FTE	%	FTE	%	FTE	%	FTE	%
Direct funding [1]	81.1	46.8	78.5	46.4	76.6	46.2	71.7	44.3	81.2	43.8	87.3	40.6
Sectorplan (via local funding)					0.6	0.4	6.1	3.8	11.7	6.3	14.6	6.8
Gravitation ICI (via local funding)									0.2	0.1	3.1	1.4
National research grants [2]	68.6	39.6	65.2	38.5	64.1	38.7	57.4	35.5	54.5	29.4	62.6	29.1
EU research grants [3]	12.0	6.9	8.6	5.1	6.4	3.9	12.1	7.5	24.9	13.4	33.2	15.4
Contract research [4]	11.7	6.7	17.0	10.0	18.1	10.9	14.5	9.0	12.9	7.0	14.4	6.7
<b>Total funding</b>	<b>173.4</b>	<b>100.0</b>	<b>169.3</b>	<b>100.0</b>	<b>165.8</b>	<b>100.0</b>	<b>161.8</b>	<b>100.0</b>	<b>185.4</b>	<b>100.0</b>	<b>215.2</b>	<b>100.0</b>
<i>Expenditure:</i>	<i>k€</i>	<i>%</i>	<i>k€</i>	<i>%</i>	<i>k€</i>	<i>%</i>	<i>k€</i>	<i>%</i>	<i>k€</i>	<i>%</i>	<i>k€</i>	<i>%</i>
Personnel costs	10,428	72.2	10,450	75.4	10,047	71.8	10,294	59.0	11,227	69.6	13,063	72.1
Other costs	4,012	27.8	3,418	24.6	3,951	28.2	7,151	41.0	4,901	30.4	5,045	27.9
<b>Total expenditure</b>	<b>14,440</b>	<b>100.0</b>	<b>13,868</b>	<b>100.0</b>	<b>13,998</b>	<b>100.0</b>	<b>17,445</b>	<b>100.0</b>	<b>16,128</b>	<b>100.0</b>	<b>18,108</b>	<b>100.0</b>

FTE: personnel employed by the University or by FOM

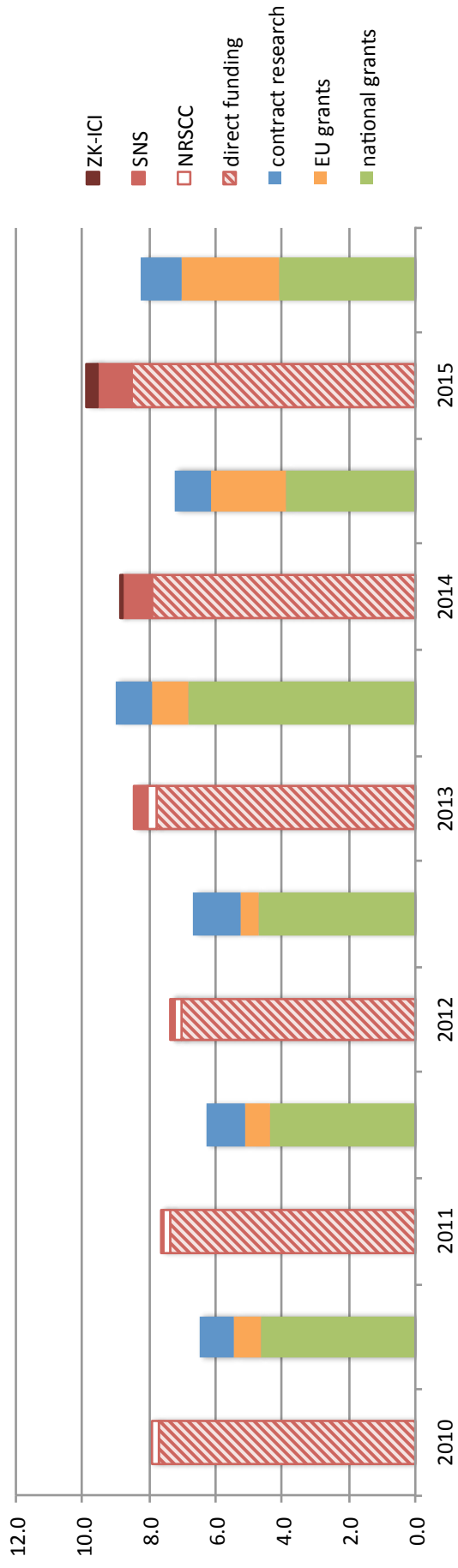
Note 1: Direct funding (basisfinanciering/ lump-sum budget)

Note 2: Research grants obtained in national scientific competitions (e.g. grants from NWO, STW, FOM and KNAW)

Note 3: Research grants obtained in European scientific competitions

Note 4: Industrial collaboration, research grants obtained from foundations and research grants obtained in other research competitions (e.g. FES, NIH, HFSP)

Chart 3: Funding sources



### 3. Research output and quality indicators

Table 3: Research output per research area and total

<b>Chemical Biology</b>	2010	2011	2012	2013	2014	2015
Refereed articles	93	87	81	82	100	86
Books	1	-	-	-	1	-
Book chapters	3	11	7	2	6	1
PhD theses	8	12	15	12	13	6
Patents	3	6	1	1	1	3
<b>Total</b>	<b>109</b>	<b>114</b>	<b>104</b>	<b>99</b>	<b>123</b>	<b>96</b>

<b>Energy &amp; Sustainability</b>	2010	2011	2012	2013	2014	2015
Refereed articles	102	92	72	95	75	72
Books	-	-	-	-	1	2
Book chapters	3	2	5	7	1	1
PhD theses	9	5	3	8	3	8
Patents	1	1	-	4	1	2
<b>Total</b>	<b>116</b>	<b>100</b>	<b>81</b>	<b>113</b>	<b>81</b>	<b>85</b>

<b>LIC Total</b>	2010	2011	2012	2013	2014	2015
Refereed articles	195	179	153	177	175	158
Books	1	-	-	-	2	2
Book chapters	6	13	12	9	7	2
PhD theses	17	17	18	20	16	14
Patents	4	7	1	5	2	5
<b>Total</b>	<b>225</b>	<b>214</b>	<b>185</b>	<b>212</b>	<b>204</b>	<b>181</b>

Not included:

Non-refereed articles, abstracts, conference papers, lectures, editorships, posters

#### 4. PhD success rate and duration

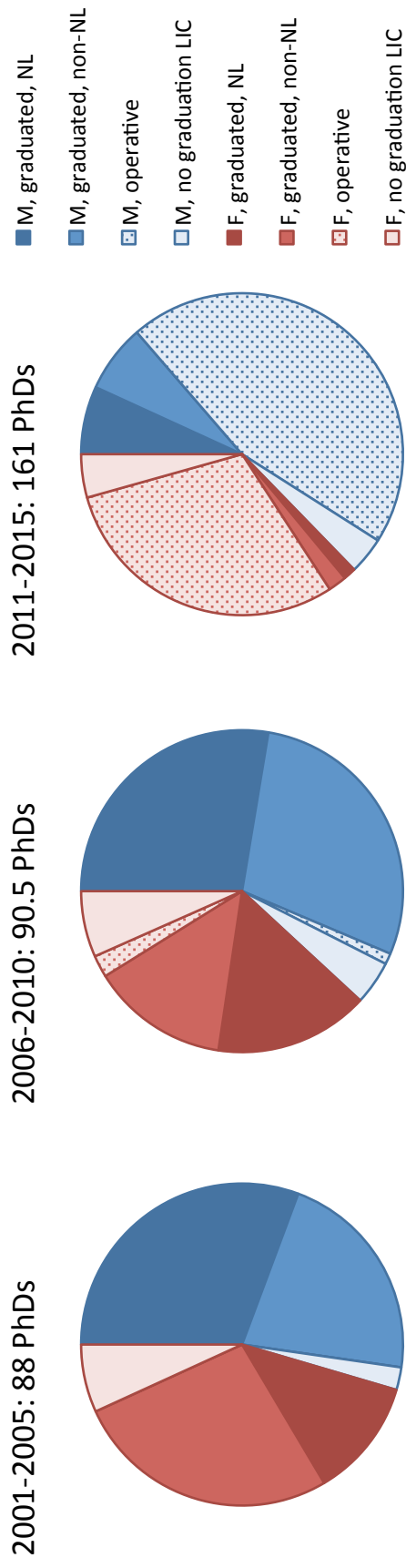
Table 4: PhD candidates, duration and success rates

Enrolment [1]		Success rates									
Starting year	Enrolment (male/female)	Total (M+F)	Graduated in year 4 or earlier	Graduated in year 5 or earlier	Graduated in year 6 or earlier	Graduated in year 7 or earlier	Graduated after 7 years	Not yet finished	Discontinued [2]		
2006	11	13	0 / 0.0%	8 / 61.5%	12 / 92.3%	12 / 92.3%	0 / 0.0%	0 / 0.0%	1 / 7.7%		
2007	13	18	1 / 5.6%	10 / 55.6%	13 / 72.2%	15 / 83.3%	0 / 0.0%	0 / 0.0%	3 / 16.7%		
2008	8	16	0 / 0.0%	12 / 75.0%	14 / 87.5%	15 / 93.8%	0 / 0.0%	0 / 0.0%	1 / 6.3%		
2009	16	30.5	1 / 3.3%	20 / 65.6%	23,5 / 77.0%	24,5 / 80.3%	1 / 3.3%	2 / 6.6%	3 / 9.8%		
2010	8	13	0 / 0.0%	8 / 61.5%	10 / 76.9%	10 / 76.9%	0 / 0.0%	1 / 7.7%	2 / 15.4%		
2011	15	21	1 / 4.8%	14 / 66.7%	15 / 71.4%	15 / 71.4%	0 / 0.0%	3 / 14.3%	3 / 14.3%		
<b>Total</b>	<b>71</b>	<b>111.5</b>	<b>3 / 2.7%</b>	<b>72 / 64.6%</b>	<b>87.5 / 78.5%</b>	<b>91.5 / 82.1%</b>	<b>1 / 0.9%</b>	<b>6 / 5.4%</b>	<b>13 / 11.7%</b>		

Note 1: All PhD students with employee status and contract PhD candidates without employee status, receiving external funding or university scholarships, who are conducting research under the authority of the institute with primary aim of graduating are included.

Note 2: All PhD students that left in probation time, after year-1 (negative continuation advice), with supervisor to other university, for other reasons are included.

Chart 4: PhD candidates, five-year interval gender and nationality analysis



Absolute number of PhD students almost doubles between starting year periods 2006-2010 and 2011-2015.  
 Ratio Male/Female drops slightly from 55%:45% (2001-2005) to 62%:38% (2006-2010), to remain constant in the next period 63-37% (2011-2015).  
 Ratio graduated Dutch M/F increases from 72%:28% (2001-2005) to 64%:36% (2006-2010).