Expert report, panel 3

KTH's Research Assessment Exercise (RAE) 2021

Panel chair:
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Introduction

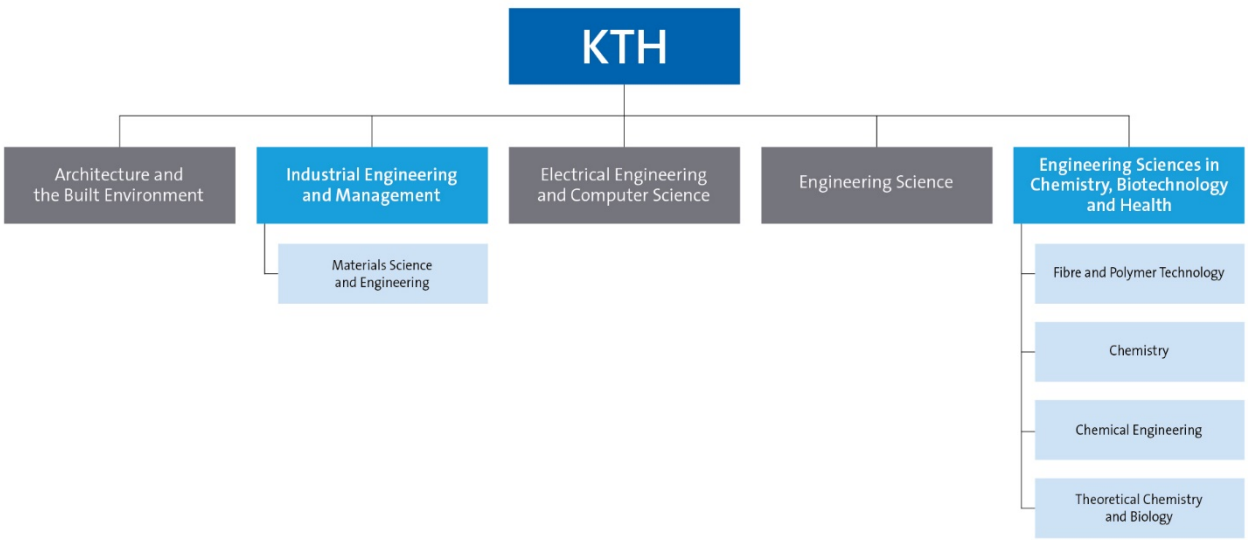
This expert panel report is part of the Research Assessment Exercise (RAE) 2021 at KTH Royal Institute of Technology. The report is based on the self-evaluation on panel 3 and aims to provide recommendations and feedback to the involved departments and KTH.

Expert panellists:

- Professor Heikki Tenhu, University of Helsinki, chair
- Professor Rasmita Raval, University of Liverpool
- Professor Annick Hubin, Vrije Universiteit Brussel
- Professor Marcel Somers, Technical University of Denmark
- Dr. Rose-Marie Fälling Yttergren, Höganäs AB
- Professor Andreas Dreuw, University of Heidelberg
- Professor Philippe Poulin, CNRS, University of Bordeaux
- Professor Anne-Marie Hermansson, Chalmers

Panel 3

Coordinator: Prof. Christofer Leygraf, KTH Royal Institute of Technology
Vice-coordinator: Prof. Minna Hakkarainen, KTH Royal Institute of Technology



Part A: Summary of the whole panel

1. Strengths, weaknesses, and recommendations

Common to the departments within the research area covered by the panel

Discussions with five departments indicated that KTH may be congratulated for its dedicated, hard-working, and motivated faculty members and researchers. Leadership works well on the department level. High collegiality in departments, divisions, and laboratories is visible. Students seem to be proud of being at KTH.

Research in the departments is application driven fundamental research. The number of industrial contacts in different departments naturally varies, but we can see fundamental and applied research being in good balance. Departments are well networked within academia and with industry, both nationally and internationally. The departments show high societal impact: chosen research topics are relevant and the students graduating at KTH are highly valued in industry.

The available instrumentation, whether located in the departments or different centres, is excellent. It is noteworthy, however, that most of the instruments lack operators. Very often PhD students are responsible even for large instruments. This may be advantageous as a part of the PhD training but carries a risk of discontinuities in the operations. The maintenance and upgrading of the instruments is problematic because no funds are allocated to such expenses. Overall, the very low number of technical staff in the departments is surprising.

The heavy, slow, and expensive top-down administration poses faculty members an increasing burden. The administrative burden is on the tipping point and severely threatens research and teaching.

There is a high potential for more collaboration between the departments and divisions. Indeed, some identical subjects are approached by the departments with different perspectives but with the same objectives. We strongly recommend KTH provides financial means to organise interdisciplinary workshops.

2. Feedback on the formulated visions and strategies

That can lead to increased quality of research at KTH and increased impact

Departments have well formulated challenging visions. Roadmaps to realise the visions would be most useful, a matter which has already been discussed, however, it seems hard to find time and space for creating these. Economic and time limitations complicate long-term planning. Excellent research is done in the departments, and collaborations between them should be done in a coherent way. A way out could be to provide faculties extra base funding for a team which drafts the roadmaps for selected cross-departmental areas.

3. Ideas and recommendations for essential steps

To be taken to renew research areas

To increase the quality and impact of research we suggest KTH considers open calls to hire excellent scientists. To attract top-level scientists and to keep them, conditions for research also need to be excellent.

Recruitment processes are too slow. Several good candidates have disappeared because of this. Rethinking of the process is necessary, and care should be taken in the selection of professor candidates and needs to be done on the department level.

4. Potential links and synergies

Between the departments within the research area covered by the panel and other parts of KTH

As already pointed above, there is a strong potential for collaborations between departments and divisions. To create cross-cutting research, organising interdisciplinary workshops should be supported, as also brainstorming to sketch the future roadmaps. It is clearly observable that collaborations between theoretical and experimental groups have a great potential to be strengthened.

Because the research in chemistry and materials has strong societal impact, partnerships with the researchers in economics and social sciences could turn out to be beneficial, in particular in the frame of sustainability goal of KTH.

Several departments produce considerable amounts of data. Data management should be taken care of, obviously on KTH level. This is a prerequisite for creating data driven research.

5. Recommendations for strengthening the departments and their future potential

The relevant points have been given already above and will be discussed in the next section.

6. Recommendations applicable to the whole of KTH

A surprising matter, which clearly hampers research is too low base funding for departments. This came out in all discussions and it seems obvious the funding is not competitive even in Sweden. The distribution of funds to the departments and divisions should be transparent.

The administration at KTH is slow and expensive, and works top-down. This increases the workload for the faculty members. Clear processes must be defined and implemented to support needs of both central administration and faculties. Faculties should be involved in the development of the administrative processes.

Overheads paid to the central administration and schools, as well as the cost of premises are prohibitive. A review process is recommended to identify and implement feasible cost reductions. The overheads should be made transparent, allowing the departments to see what they pay for. Owing to the circumstances, hiring a PhD student is very expensive and in several fields the number of students has been decreasing. Cost reductions indeed are necessary.

The recruitment processes are far too slow and measures need to be taken to make them more straightforward. As already noted above, the selection of professor candidates should be done on the department level.

Part B: Report for each department

Department of Fibre and Polymer Technology

Major findings

1. Strengths and weaknesses of the department

Concerned and recommendations for improvement

A strong department consisting of seven divisions, all working on various aspects of polymer science and technology. Importantly, both biopolymers and synthetic polymers and materials are gathered in the same department.

The strengths identified by the department are: research in both fundamental and applied science, as well as experimental and modelling research; strong scientific culture with broad coverage of macromolecular science, including both natural and synthetic polymers; strength in fundamental research allows to address applications of choice; strong long-term external funding; critical mass to perform advanced interdisciplinary research; large instrument park available for the entire department. The department has received a high number of advanced research grants, nationally and internationally. The department is involved in broad national and international network in academia and industry, and actively collaborates with large infrastructures as DESY and MAX IV.

Main weaknesses identified by the department are economic and administrational. In general, it is difficult to support in-depth narrow research fields. Strong long-term external funding is essential for the research activities but the lack of full coverage of overheads on external funding erodes the faculty funding. The base funding for faculty members is weak and constant raising of money for own salary and for PhD students and postdocs takes focus from research. Maintenance and upgrading of the infrastructure are expensive. On the organisation side, the identified weaknesses are: too lengthy recruitment procedures, which sometimes lead to the disappearance of good candidates; limited administrative support on department and division level; too slow processes to adapt facilities, e.g. laboratory renovation/adaptation; too weak support with managerial duties with large research centres, faculty members use too much time on administration; administration on the university and faculty levels is costly, which results in high overheads. It is also noted that the leadership positions are not awarded; they come at the cost of academic career and thus are often avoided.

The department is the largest academic institution on macromolecular science in the Nordic countries. Fundamental and applied research are in harmonic balance, however, too low base funding limits all activities. The department is well networked in academia and with industry, both nationally and internationally. The engagement in large international research consortia is considerable, and this is strongly supported by the panel. For further strengthening of the department, it is vital to keep the balance between fundamental and applied research.

The high societal impact of the department is seen in extensive connections with industry, in the high number of advanced research grants nationally and internationally, and in the numerous spin-offs and products. The department aims to identify the ways of increasing its visibility within the scientific community and in society in general.

2. Relevant and forward-looking objectives

Are the goals relevant and forward-oriented?

The vision of the department is to provide the society with “sustainable macromolecular materials – from molecules to macroscopic assemblies and devices”. This is realised through research objectives which cover essential fields of macromolecular science from the synthesis of monomers (building

blocks of polymers) to polymer technology and chemistry of natural polymers. The goals of research are highly relevant and forward-looking.

3. International community engagement

The department is well networked in academia and with industry, both nationally and internationally. The engagement in large international research consortia is considerable. Wide range of competencies ranging from paper and pulp technology to polymer chemistry and fibre technology together with well-equipped facilities have made the department an attractive partner in international collaborative research projects, both with industry and academia.

4. Future potential of the department

The department is very strong and capable of fulfilling its goals. Activity in fundamental research and increasing involvement in large research consortia makes it possible to act in the front line of international research. The department is also oriented towards interdisciplinary research. This can be seen for example in the Wallenberg Wood Science Center, which is truly interdisciplinary and presents an outreach from a traditional industrial area (wood-based materials) toward new uses, applications and concepts, i.e., to other fields. Growing involvement in energy related research projects is another sign of interdisciplinary work. Developments in the fields of energy, medicine, renewable materials, nanostructured materials, and multifunctional materials and devices present a huge future potential.

5. Recommendations

Obviously, better base funding and less administrative burden are the keys to further develop the department. Strong fundamental research has made it possible to tackle in applied projects, which are found relevant in sense of the research programme. Some examples of high risk-high gain research are transparent wood and battery research. Interestingly, lignin (a wood component that many generations of chemists in the Nordic countries have studied) has turned out to be a source for new materials. Continuous investment in fundamental research is important for the future.

The present infrastructure, i.e., the modern research instruments, is good and made available for everyone in the department. Measures need to be taken to secure the maintenance and upgrading of the instruments in the following years.

The seven divisions are not equally strong what comes to the number of permanent staff. This may be a matter to be further discussed. At the moment the number of young assistant and associate professors is low because of several recent promotions. This is a good sign of preparing for the future but also poses a question of a need for new recruitments in coming years.

Specific issues

1. Research profile and quality

a. Central research questions and themes, and main research activities

The vision of the department is to provide the society with “Sustainable Macromolecular Materials – from Molecules to Macroscopic Assemblies and Devices”.

The department comprises seven divisions: Polymer Technology, Polymer Materials, Coating Technology, Fibre Processes, Fibre Technology, Biocomposites, and Wood Chemistry and Pulp Technology. The department also hosts the Wallenberg Wood Science Center funded by KAW. The unique niche of FPT is the combination of chemistry, physics and mechanics of synthetic and native polymers (mainly wood based) including fundamental science and applied research.

For the *Division of Biocomposites,* the focus area is nanostructures polymers, where at least one of the components is of biological origin. Characterization of nanostructure, experimental mechanics and molecular dynamics simulation are important areas of competence. The profile of the *Division of Polymer Technology* is design of stable and degradable polymers considering the principals of green chemistry and the whole life cycle from raw materials to end-of-life management. One focus is functionality and interactions of the materials in targeted applications and controlled long-term performance or programmed degradation. The work at the *Division of Fibre Technology* is focused on molecular tailoring of cellulose fibres and fibrils and a fundamental characterization and understanding of the colloidal and chemical behaviour of cellulose nanofibrils.

The *Division of Polymers Materials* has the motto to establish relationships between structure and properties ranging from fundamental research, involving theory, simulation, modelling, advanced experimentation to more applied research. The profile of the *Division of coating technology* is new materials based on renewable resources, polymer modelling, processing, nanostructured polymeric systems, insulating polymeric materials and long-term performance of polymeric materials. One focus is he interplay between macromolecular architecture and macroscopic properties applied to thin polymer films. The research is synthesis- oriented with expertise in monomer synthesis, polymerizations, macromolecules with complex architecture as well as enzymology and biocatalysis. *The Division of Wood Chemistry* and Pulp Technology deals firstly with steps involved in processing wood to pulp fibres and as well as the chemistry involved and secondly with the morphology, chemistry and biology of wood and its products. On-going work deals with the modification of the pulping processes and new ways of isolating, functionalising and using wood polymers in materials and energy applications. Recently the department has been expanded with the new Division Fibre Processes, with the aim of strengthening making this possible to really implement this concept into new materials. A specific contribution research and education on processes for material fabrication from wood fibres forest resources. The research topics ranges from developments of the industrial processes for paper and packaging manufacturing, to new processes and industrial fabrication processes of novel materials based on wood-pulp fibres and nanocellulose. A central part in these developments is the use of characterization techniques based on synchrotron radiation and neutron scattering.

b. Contributions to the advancement of state of the art within the research fields of the department

The combination of advanced polymer synthesis with advanced characterization methods and novel applications enables sustainable material solutions. The development in the forest and agricultural area towards a biorefinery concept coincides with a strong demand for biobased monomers from the traditional polymer industry. New materials are continuously developed for different application areas. The research at FPT strongly contributes to multiple fields. This can clearly be seen in the bibliometric evaluation where the data show a strong impact in an international comparison. An evolving field relates to scaling factors where the nano-meter range has obtained a significant interest during the last

decade. The concept of designing of structures on a nanometer scale has been demonstrated to have a significant impact on the materials performance. Several components such as inorganic nanoparticles, carbon tubes, graphene, and nano fibrillated cellulose (NFC) are now available as starting materials for to the advancement of state of art from relates to transparent wood, which has been expanded into wood nanoscience and nanotechnology. This represents a top-down approach to cellulosic nanomaterials with multiple functionalities. Regarding medical applications collaborations exist between researchers at FPT and Karolinska Institute Materials for medical applications range from range from targeted drug delivery using dendritic polymers to polymer scaffolds for implants and tissue engineering. Energy distribution and storage are key areas in for a sustainable society. Distribution and storage of energy, will materials range from irrespectively of the energy source, be needed to obtain an efficient energy use. New macromolecular electrical cable insulation materials to membranes for fuel cells or solid polymer electrolytes for batteries.

c. Quality and quantity of contributions to the body of scientific knowledge, engagement in national and international research collaboration within academia and its outcome

FPT have a very strong position at KTH by its leading role in the Wallenberg Wood Science Centre (WWSC). It is a joint research center at KTH, Chalmers, and LiU which aims to build a research program on new materials from trees. The program is highly multidisciplinary, and is developing technology platforms as part of the strategy. WWSC was established in 2009 with funding for a 10-year period. In 2019 was the center renewed (WWSC 2.0) for an additional period of 4+6 years with a total funding of 700 MSEK. WWSC has a strong impact on national collaboration both with academia and industry. It is also important for internal collaborations within KTH, which is mentions in the self-evaluations of other departments

FPT also hosts several highly ranked international scientific journals with FPT faculty/staff as Editor in Chief or Editor. Several faculty/staff members also serve as board members and guest editors in numerous international scientific journals. Recent previous engagements include journals such as Biomacromolecules (Founding editor and editor-in-Chief Ann-Christine Albertsson), European Polymer Journal (Editor Ulf Gedde), and Polymer Bulletin (Editor Eva Malmström). Faculty at FPT has also written seminal textbooks within the research field that has reached global attention e.g., “Fundamental Polymer Science”, U. W. Gedde, M. S. Hedenqvist, Springer, 2019. Faculty of FPT has contributed with a large number of invited plenary and keynote talks, assignments as editors, memberships in research councils, learned societies, and serving on evaluation committees for research councils and faculty positions, both domestically and internationally. Leadership shown as project coordinators for research programs of considerable size is also found at FPT.

d. Follow-up from previous evaluations

- *RAE2012: The high amount of short-term funding of research is a continuous concern and some increase of the basic funding is needed.* The situation has not changed. Faculty funding does not cover salaries of faculty members and constant efforts to raise money to cover own salary and costs for PhD students, overheads co-funding etc. takes focus from research
- *RAE2012: Incentives to increase and enable more interdisciplinary work within KTH ought to be considered, e.g., specific funding of joint projects.* Incentives to increase and enable more interdisciplinary work have improved considerably by several large research programs such as WWSC, MISTRA TerraClean, BiMaC Innovation, Treesearch, FORMAX. By leading large centers FPT can initiate cross-cutting research between departments as well as between other universities
- *RAE2012: Possibilities to hire technical staff to support in maintaining and use of measurement equipment’s must be explored.* In general, the lack of technical staff is still a problem. However, one scientist has been allocated to support advanced microscopy (SEM, TEM)
- *RAE2012: Patenting and innovation activities ought to be strengthened through education and networking with industry*. These activities have increased significantly.

2. Viability and research environment

a. Internal and external funding; current status and strategies for the future

The department is internally underfinanced. The base funding for faculty is low and does not cover salaries. The already very low internal funding is eroded since the external funding (especially from foundations) does not cover the high costs for overheads and premises and the only source to cover this is the internal funding. Also, the undergraduate education at KTH is heavily underfinanced on a departmental level. Thus, the research is to a large extent externally financed. The researchers at FPT are very active in searching research funding and attractive as research partners and have a good success rate in funds applied for. A large fraction of FPT´s external funding has a long-term perspective i.e., projects with a life time of 5 years or more (e.g. WWSC, ERC, KAW, etc.). The department is very strong in funding from foundations (e.g., KAW) and less successful in retrieving funding from EU. This is clearly something that the department can develop further, i.e., try to get more EU-funding.

b. Academic culture

The academic culture is very good. In the interviews it came out, that faculty and students on all levels think the department is a great place to work. There are no barriers, and the young faculty are welcome to discuss with their peers without any formalities. There seems to be good interactions across research groups in the department. The faculty arranges PhD courses open for all students that try to address a broader perspective into the research field. Open meetings on common research themes were recently founded as a tool to promote an enhance a sound academic culture e.g., regular meetings between divisions on the field of lignin research were established last year. These informal groups are good initiatives to reach out for collaboration outside the department.

c. Current faculty situation and composition of the research team(s)

The balance between professors and junior faculty shows some overweight towards professors. There is room for more assistant professors. According to the self-evaluation report there is only one assistant professor, but there has been a recent promotion to associate professor. Two senior professors in cellulose and cellulosic materials are approaching retirement. The recruitment of adjunct professors is seen as a strategically important way to connect complementary disciplines to the department for a more interdisciplinary research approach. These recruitments also allow for strategic alliances to be formed with external partners. There is a decrease of PhD student in favour of postdocs There is a large group of researchers and postdocs that are externally finances. The balance between faculty and researchers needs to be considered.

d. Recruitment strategies

FPT can attract good scientists and should be encouraged to really go for excellence when recruiting young faculty in very open calls, that can have a bearing on new developments within the department. However, good conditions must be offered to be attractive on an international level. Not only competing universities but also industries are aware of the need for competences within fibre and polymer technology. FPT have been successful in recruiting talented graduate students for all over the world. The possibilities for researchers to apply for a faculty position need to be clarified.

e. Infrastructure and facilities

FPT is well equipped. The infrastructure and instrument facilities at the department are based on an instrument park available to all researchers at the department. This can be developed further to embrace the whole school and initiatives have been taken in this direction. A common infrastructure will promote cross-cutting research between departments. One of the main challenges is to find funding for maintenance and up-grading of the present instrument park. There is also a lack of funding

for technical staff to support the infrastructure. FPT has also established collaboration with large national and international advanced research facilities to enable availabilities to these facilities

3. Strategies and organisation

a. Goals for development 5–10 years ahead

The vision of the department is to provide the society with “Sustainable Macromolecular Materials – from Molecules to Macroscopic Assemblies and Devices”. The department aims to continue to be a globally leading actor on this topic within the strategic research areas (life science, energy, renewables, nanomaterials, multifunctionality, and devices).

The short-term missions of the vision are clear but on the long term the department is dependent on the external funding situation. A roadmap, especially for crosscutting research is recommended, where FPT can take the initiative based on their leading role in big centres like the WWSC.

b. Congruence with university-level goals

The goals of the department are in line with the KTH development plan. The vision of the department is very much in line with KTH ´s development plan on a “A leading KTH” especially for a sustainable society. Most research at FPT relates to this and thus add to the overall sustainability approach of KTH. However, the communication links between the top management and the departments are not very clear and no information of interactions between the department, the schools, vice presidents and the vice chancellor has been given.

It has been pointed out that the administrative and economical constraints are bound to affect the quality and motivations. With better base funding and less unnecessary administration, the work environment would improve, and it would be possible to spend more time on what professor should do, i.e., teaching, research, and outreach. This would contribute to a leading and more visible KTH.

c. Leadership structure and collegial structure

The leadership is very good and there is a high motivation for a collegiality driven organization. The young faculty, especially from abroad appreciates the academic freedom at KTH. FPT have an advantage that the competences between the divisions are complementary for the area of fibre and technology, which promotes communication between divisions.

The formal leadership is organized according to a conventional line organization. The department is organized with seven different divisions each with a division head. The heads of divisions and the head of department form a department management team coordinates all activities. However, it was not clear to the panel how and in which way, the heads of the department communicate with the schools and the central administration. The panel understood the links to the central administration are one way and top down, which is unfortunate.

d. Strategies for achieving high quality

The majority of all scientific publications are published in open access and in relevant, high- impact journals. The success to attract prestigious grants and findings for establishing centers like the WWSC is both a measure of quality and a prerequisite to maintain high quality. International and national collaboration and interchange are considered of importance to remain relevant to the scientific community. An important task is the training of PhD students into good scientists and leaders in academia and industry.

4. Interaction between research and teaching

a. Interaction between research and teaching at all three levels (B.Sc., M.Sc., Ph.D.) of education

All faculty members at FPT are involved both in research and teaching on all levels. The research also connects to all levels of education in several ways. Teachers on undergraduate level that are active in research can bring relevant practical examples into the course material and thus up-date course content. Master theses-, Bachelor theses-, and project course students work closely with PhD-students and postdocs, often in combination with industry. PhD-students also get training in supervising undergraduate students as a part of the PhD program.

It was stated that the undergraduate education at KTH is heavily underfinanced on a departmental level. It is not clear if that influences quality of the teaching. Also, the decreasing number of PhD students could be a threat to the teaching in the long-term perspective as they are involved in the teaching of undergraduates.

5. Impact and engagement in society

a. Relevance, scale, and impact of the department's current engagement with society and industry

The forest-based industry has boosted the development of application driven basic research in Sweden. Without their engagement, platforms like Treesearch and Centers like WWSC as well as VINNOVA Centers would not exist. Know how from research is transferred to industry in research programs and by patent rights and in some cases as start-up companies. The forest-based industry, polymer industry, and to an increasing extent, other users of macromolecular materials as developments in many fields ask for new advanced materials, e.g., the energy field. The strong collaboration with external partners has a direct impact on the educational program through e.g., MSc thesis works conducted in industry and internal and external PhD projects funded and co-supervised with industrial partners. The strong interaction with the surrounding society ensures that the students at both advanced and graduate level obtain relevant training for their future employments. Another route of knowledge transfer is the transfer of trained staff from FPT to industry the society. This is dominated by MSc´s and PhD´s that take up positions throughout society after obtaining the degree.

FPT conducts research that is relevant for a multitude of societal needs (energy, medtech, bio-based (sustainable) materials, transportation sector, therapeutics, nanomaterials, packaging materials). In the transition to a sustainable society, PFT is recommended to extend its engagement in society, along the lines described below, by addressing the general public as well as politicians and demonstrate the important role of application driven science.

b. Research dissemination beyond academia

The following examples are given in the self-evaluation report. Personnel from FPT actively interact with high schools are by hosting visits for students and teachers as well as giving talks at various high schools. Researchers from FPT also regularly give popular scientific presentations at a range of events open to the public e.g., talks at the Nobel museum, the Technical museum, "forskarfredag", IVA-seminars, branschdagar (SPCI), and at the research school in Karlskoga. Other involvements include presentations in various media such as TV, Radio, Twitter, and Facebook. Staff members from FPT are actively participating in Tekla-days at KTH, House of Science (Vetenskapens Hus), Tom Tits, and also hosting children and youngsters as well as business leaders and innovators for study visits. School children come for their PRAO at the department. Research results from FPT is also announced via press releases aiming towards a broader audience.

c. Relation to sustainability and the United Nations' Sustainable Development Goals (SDGs)

The relations to sustainability are convincingly outlined in the self-evaluation report. A significant share of all research projects is now focused on the elaboration of more sustainable materials and material concepts. New material solutions are needed in several of the UN´s goal for future sustainable societies. These range from improved Health (e.g., medical devices, implants, and diagnosis) to sustainable Energy solutions (e.g. energy storage, energy distribution, and energy harvesting), and renewable resources (e.g. forest and agricultural sources). An estimate is that +80% of the research at FPT has relevance for the SDGs, directly or indirectly.

d. Plans and structure for increased impact

The department is in a good position to further strengthen impact through the National platform Treesearch and the involvement in research Centers focussed on forest-based product and processes. It is recommended that they continue to develop this structure also when it comes to other material concept for sustainable materials. In this context, the potential of cross-cutting research between departments on selected areas can increase the impact of KTH.

6. Recommendations for strengthening the department and its future potential

The department is world leading in many fields of polymer and fibre technology and there are synergistic links between the divisions. The panel´s recommendation is to continue to strengthen the high scientific level as well as the strong relations with the industry in the following ways.

- There is a long tradition to work with the forest industry and their needs. This can be expanded and transferred to new material demands and other industrial constellations. It is recommended to continue to develop centres/platforms with new applications.

- There is an overweight towards professors and a need to strengthen the young faculty. FPT has the reputation necessary to attract assistant professors based on excellence. Therefore, open calls are recommended, that can pave way up for new developments within the department.

- An important impact is PhDs employed by industry after graduation. It is worrying that the number of PhDs are decreasing in the favour of postdocs. The panel recommends a revision for the costs of PhDs.

- The panel recommends FPT to continue to take initiatives for cross-cutting research between departments at KTH and make a roadmap for selected areas, where seed money should be provided. *Already in RAE2010 it said that; Incentives to increase and enable more interdisciplinary work within KTH ought to be considered, e.g., specific funding of joint projects.* Some progress has been made and it is clear that FPT can take a leading role. Increased collaboration and synergistic effects can be achieved with for example the departments of chemistry and theoretical chemistry.

- FPT is recommended to continuously develop and upgrade its instrumental facilities in an infrastructure available for the entire school. For advanced instrumentation skilled technical staff is needed that can run the instruments but also help with experimental design and evaluations. This was a recommendation already in RAE 2012*: Possibilities to hire technical staff to support in maintaining and use of measurement equipment's must be explored* and since then one scientist has been allocated to support for electron microscopy.

- Better base funding and less administrative burden are the keys to further develop the department. This was already pointed out in RAE2012 and the situation seems to have become worse. (*RAE2012: The high amount of short-term funding of research is a continuous concern and some increase of the basic funding is needed).* We can already see the effects of overhead in the decreased number of PhD students and difficulties to recruit the best scientists.

7. Final remarks

We lack information from the schools, where decisions of importance for the developments are being made as far as we understand such as decisions about young faculty recruitment, seed money etc. There are also many weaknesses regarding central administration, which seems to be a top-down process. From departments it was e.g., claimed that the recruitment process was far too slow and that there is an increasing burden from the administration

Department of Chemistry

Major findings

1. Strengths and weaknesses of the department

Strengths:

The Department of Chemistry has a broad and inherently interdisciplinary and diverse scientific base that enables it to conduct research and teaching across a range of fundamental and applied areas. The department is grouped under four main divisions: Organic Chemistry, Applied Physical Chemistry, Surface and Corrosion Science, and Glycoscience. The department has excellent research infrastructure and facilities, further augmented by the acquisition of XPS and nano-IR instruments and the creation of the 2MILab with advanced equipment that is accessible to the whole school.

Overall, the department contributes significantly by delivering excellent research, teaching, international profile and impact (research, societal, industrial) that is commensurate with KTH's position at Sweden's largest technical university. Sustainability goals are embedded in the departmental strategy and outputs. There is a high degree of academic talent and real commitment to excellence and inter-division collaboration. Overall, the department is delivering internationally leading/competitive science. The department has a healthy output of research papers across all divisions, including a good number of high impact publications in the Nature group journals, Angewandte Chemie, JACS, PNAS, etc.

There is clear evidence that the department is run very well with real leadership and a high degree of collegiality, inclusivity, consultation, mentorship and support. This aspect was very impressive and delivers a high functioning department and engenders a positive and welcoming working environment for researchers and staff at all levels. It is a key factor in retaining high morale, motivation and institutional loyalty. Young faculty can operate with research independence within a supportive and collaborative environment that allows talent to be nurtured and developed.

The Department of Chemistry carries the largest teaching burden in the School, with all academic staff involved. There is a direct and positive connection between research and teaching at all levels, exposing students to state-of-the art knowledge in specialist areas. This integration between research and teaching is commendable and underpins the department's success in producing graduates that are highly prized and sought after by industry. Sustainability is an important thread running through teaching and research and this aspect is particularly attractive to students.

The department has created high impact with society and industry in a number of areas. First and foremost, it creates skilled graduates and PhDs who are highly prized by industry. There are also close ties between individual researchers and 100+ industries, with a number of sponsored PhDs, collaborative projects and contract work, thus translating academic knowledge into the technological sphere. Some faculty staff also hold part-time positions in companies. The exemplar impact cases provided in the self-evaluation were impressive. Departmental research has led to spin-out companies.

Weaknesses:

The department faces a critical situation regarding the internal funding model, which has decreased in relation to costs. This unfavourable financial environment places a huge burden on the faculty, which is forced to work on a survival strategy, with almost no 'breathing space' required for developing and implementing long term strategies and funding plans. Thus, the current financial burden placed on staff is significantly eroding the ability sustain research and impact at the highest level.

The department suffers from high bureaucratic/administrative demands. Insufficient administrative support is provided at the local departmental level. Whereas institutional administration resources should alleviate academic workloads, KTH's administration and processes are cascaded downwards and are significantly increasing academic burden, leading to high stress and loss of research time.

Six faculty members will reach retirement age within 5-10 years and replacements will need to be planned to allow the department to continue functioning. Unfavourable conditions imposed at KTH have, and will continue to, result in significant talent drain of successful staff.

Recruitment into faculty positions is currently hampered by two main aspects: i) KTH does not provide competitive starting or working conditions, even in relation to other Swedish universities; and ii) KTH has a convoluted and bureaucratic hiring process, during which promising candidates are lost- this needs to change quickly.

There is no central funding allocation or formal platforms to actively channel and drive industrial contacts and engagement at the departmental level. There appears to be no effective institutional framework or direct resource to capture the breadth and depth of this impact, or indeed to reward it (e.g., via salary contribution).

2. Relevant and forward-looking objectives

Overall, the departmental goals are relevant and forward-looking. The department's teaching and research requires an inherently diverse disciplinary base, which is also geared towards impact. Sustainability remains central to future objectives. There is clear understanding of the infrastructure requirements to underpin future objectives.

3. International community engagement

The department has an active and vibrant collaboration culture at the inter-divisional, inter-departmental, national and international level. These collaborations are highly productive and 72% of the department's papers in 2016-2018, were achieved through international collaboration.

4. Future potential of the department

Looking to the future, there is a real opportunity to create synergies and increase research power by formulating inter-departmental research themes that harness complementary strengths to address grand challenges of scientific and societal importance. The panel noted potential inter-departmental connectivity in solar energy, catalysis, electrification, clean sustainable materials, surface corrosion and tribology, bio-based materials, and connecting nanolevel measurements to processes and performance in the real world.

However, academic staff will need time and space to explore and implement this and will need to be supported by the institution.

5. Recommendations

There is a real opportunity to consolidate the departmental and inter-departmental research strengths into cross-cutting inter-departmental in order to address specific grand challenges with the critical mass and research power required to create a unique leadership position for KTH. Academic staff will need time and space to explore and implement this.

Advanced science needs increasingly advanced instrumentation to remain competitive. A longer term infrastructure plan is recommended. KTH will have to consider how more permanent technical support can be enhanced at the departmental level to support this infrastructure.

Recruitment plans to replace expected academic retirements need to be implemented so that new faculty are accommodated without loss of momentum.

The current KTH financial model needs to be revised in order to safeguard departmental viability and provide the space and time for faculty to strategize, develop, and sustain future research initiatives at the highest level. It is also adversely affecting recruitment and retention of talent.

KTH central administrative culture and frameworks need to pivot towards alleviating academic workload, be more agile and efficient (e.g., in recruitment), be made available locally at the departmental level and be responsive and open to academic needs and strategy.

Impact activities should be recognised and rewarded by the institution (e.g., via salary contribution). Central funding allocation for cohesive formal platforms to actively channel and drive industrial contacts and engagement at the departmental level would be advantageous.

Specific issues

1. Research profile and quality

a. Central research questions and themes, and main research activities

The department of Chemistry has a broad and inherently diverse scientific base that enables it to conduct research across a range of fundamental and applied areas. These are grouped under four main divisions, each with specific foci of interest:

Organic Chemistry, which focuses on sustainability including solar cells/solar fuels and artificial photosynthesis, and sustainable synthesis via photoredox catalysis, electrosynthesis, and organo- and metal catalysis, supplemented by a new faculty appointment in supramolecular chemistry and molecular machines.

Applied Physical Chemistry conducts research in perovskite solar cells; metal catalysis, protein microfibres and sensors (with 2 ERC grant-holders).

Surface and Corrosion Science with focus on corrosion, friction, wear, tribology and ionic liquid and biomimetic lubricants, materials for high T applications, and advanced vibrational spectroscopic techniques e.g., nanoIR.

Glycoscience, which is highly interdisciplinary and combines molecular biology, biochemistry and material sciences to utilise nature's building blocks to create high value multifunctional carbohydrate-based materials with advanced properties.

In addition, the department hosts **the 2MI lab** with advanced equipment that is accessible to the whole school.

b. Contributions to the advancement of state of the art within the research fields of the department

The high degree of academic talent and commitment to excellence and inter-division collaboration is evident in the following notable advancements of state of the art:

Internationally leading achievements in dye-sensitized, perovskite, and quantum dot solar cells, which has culminated in high impact papers and led to the development of company Dyenamo AB, which drives development of dye-sensitized and perovskite solar cells. Additionally, work on artificial photosynthesis systems for water oxidation, catalysts for water splitting, CO_2 reduction and catalysts for N_2 fixation provide routes to solar energy conversion systems.

Another strong field of research at the division is sustainable chemistry in organic synthesis using photoredox catalysis, organic electrosynthesis, and electrochemistry.

A glycoengineering toolbox combining metabolic engineering, enzymology, biochemistry, surface modification, supramolecular chemistry and biosynthesis is helping to develop pest control strategies in aquaculture and food crops and design sustainable processes to deliver high-value products for bioplastic, food, cosmetic and biomedical applications.

Notable successes are also evident for interfacial processes with emphasis on highly local effects on corrosion, wear and lubrication, the relation between friction, surface composition and tactile perception (pyschotribology), novel lubricants, etc.

The department has also reinforced recently by two ERC grantholders who are leading efforts in advancing environmental and in situ sensors.

The department also advances the development and use of spectroscopic and imaging techniques, such as vibrational sum frequency spectroscopy, scanning probe microscopy, NanoIR, NMR spectroscopic methods to both applied basic research. The experimental effort is complemented by quantum chemical modelling.

Overall, the department is delivering international leading/competitive science. Looking to the future, there is a real opportunity to create additionally and increase research power by formulating inter-departmental research themes that harness complementarity and strengths to address grand challenges of scientific and societal importance. The panel noted potential inter-departmental connectivity in solar energy, electrification, catalysis, clean sustainable materials, surface corrosion and tribology, bio-based materials, and connecting nanolevel measurements to processes and performance in the real world. However, academic staff will need time and space to explore and implement this and this needs to be supported by the institution.

c. Quality and quantity of contributions to the body of scientific knowledge, engagement in national and international research collaboration within academia and its outcomes

The department has a healthy output of research papers across all divisions, including a good number of high impact publications that are internationally leading with high citations, including high profile journals such as the Nature group journals, Angewandte Chemie, JACS, PNAS etc.

The department has an active and vibrant collaboration culture at the inter-divisional, inter-departmental, national and international level. Highlighted collaborations include those with the Wallenberg Wood Science Centre, TreeSearch (the Swedish Infrastructure for New Materials from Trees), the Centre of Molecular Devices (CMD), STandUP for ENERGY (SfE), the Center of Artificial Photosynthesis (CAP), and collaborative networks in ionic liquids, digitalization of medicine

metal corrosion and environmental impacts, protein based materials (driven by the Department). Several staff have formal associations with leading universities in Sweden, Europe and the Asia-Pacific.

These collaborations are highly productive and it is noted that 72 % of the department's papers in 2016-2018 were achieved through international collaboration.

d. Follow-up from previous evaluations

The Department of Chemistry received an excellent evaluation (15 out of 15) in the previous RAE, with its research rated outstanding and its impact on industry, on governmental policy rated as of considerable importance. The following recommendations were made: "The potential for achieving future goals is high. Nevertheless, some improvements are possible, including providing incentives and environments for enhancing internal collaboration within KTH, and ensuring that the present balance between basic and applied science remains; "It appears that the current research topics are mostly promoted by professors or associate professors, and new research topics independently developed by young assistant professors are lacking" and "the department's GLY unit demonstrated world-leading research but the sustainability of the excellent research environment of the unit was questionable due to loss of key personnel to competing institutions without replacement."

It is evident from the self-evaluation report and panel meeting that internal collaborations have increased significantly. The department hosts advanced instrumentation facilities like the 2MILab, which has the potential to become a collaboration engine. Most of this is driven on a one-to-one collaboration basis, there is now an opportunity to strategically develop inter-departmental cross-cutting themes that bring additional synergy and research strength.

The department has recruited several people at the Assistant Professor level and, from our evaluation, it is clear that they are independent and control their research agendas, incubating new effort in chemical sensing and new research at GLY. Substantial external research grant portfolios have been established by all these appointees. 2 junior faculty appointments and 1 promotion to Professor have since been made, but may need further reinforcement. GLY's young researchers have secured large grants (SSF, VR, Formas, Energimyndigheten).

The ~50:50 balance between basic and applied science is appropriate but remains outside departmental control and subject to fluctuations in external funding and external strategic directions.

2. Viability and research environment

a. Internal and external funding; current status and strategies for the future

External funding increased significantly in 2019, with funding from the Swedish Research Council VR decreasing in importance while funding from other sources like Formas, Olle Engkvists Stiftelse, Åforsk have increased. However, external projects requiring internal co-funding from the KTH are not possible, excluding participation in national and international collaborations.

The department faces a critical situation regarding the internal funding model, which has decreased in relation to costs. A critical situation has developed with the shortfall in salary funding and the large overhead and rent costs. This unfavourable financial environment places a huge burden on the faculty, which is forced to work on a survival strategy, with almost no 'breathing space' required for developing and implementing long term strategies and funding plans. Further, as national and international funding strategies change and evolve, agility is required to maximize grant success- this cannot be effectively managed under such economically strained circumstances. The internal funding model at KTH is, therefore, a critical factor threatening departmental viability.

b. Academic culture

It was clear from the panel interview (which included a separate section to talk to younger staff and researchers) that the departmental culture is supportive, inclusive, collaborative and this is critical in driving excellence across all divisions. This is impressive and, at the departmental level, there is much to be admired about the leadership and management structures in place.

A disconnect between the department and the KTH upper management is apparent. There are high bureaucratic/administrative demands on academic staff. Little administrative support is provided at the local departmental level. In fact, KTH central administration is significantly increasing academic burden, leading to high stress and loss of research time. Those in leadership positions face high bureaucratic/administrative demands leaving little time and space to plan the future.

c. Current faculty situation and composition of the research team(s)

Although, there is a critical mass of researchers in each division, six faculty members will reach retirement age within 5-10 years and replacements are being planned to allow the department to continue functioning. The department aims to have positions at Assistant/Associate Professor levels to be announced in 2021 and 2022 and this will require School support.

d. Recruitment strategies

There are problems with recruitment at every level. Recruitment into faculty positions is hampered by two main aspects: i) KTH does not provide competitive starting or working conditions, even in relation to other Swedish universities. Thus headhunting international talent is almost impossible, and retention of existing staff is jeopardized. This restricts the Department to recruiting largely at the Assistant Professor level. Unfavourable conditions imposed at KTH have resulted in talent drain of successful staff. KTH also has a convoluted and bureaucratic hiring process, during which promising candidates are lost. This is an easy problem to solve- KTH needs to urgently streamline their process, involve the department in creating shortlists, and then accelerate external evaluation and interview. There are examples of best practice throughout the world that KTH can adopt. The recruitment of PhD students is now hampered by their very high cost, with postdoctoral recruitment finding favour.

e. Infrastructure and facilities

The department has excellent research infrastructure and facilities, further augmented by the acquisition of an XPS and nano-IR instrument. The creation of the 2MILab will enable co-location of advanced facilities. Access to other shared facilities at KTH also enhances research. However, there is some concern that workhorse techniques like NMR spectroscopy and dedicated mass spectrometry that are currently available on campus may be levered into national facilities, hampering research activity. Advanced science needs increasingly advanced instrumentation to remain competitive. A longer term infrastructure plan on maintaining key facilities and acquiring new equipment will be necessary and will require funding from mixed sources. The majority of the infrastructure is run by PhD students- KTH will have to consider how technical support can be financed at the departmental level.

3. Strategies and organisation

a. Goals for development 5–10 years ahead

The department's teaching and research requires an inherently diverse disciplinary base, which has to be tensioned against creation of critical mass to make scientific impact. Thus, breadth and depth need to be secured to deliver high quality of research and education.

Overall, the departmental goals are relevant and forward-looking. The department's teaching and research requires an inherently diverse disciplinary base, which is also geared towards impact. Sustainability remains central to future objectives.

There is a real opportunity to create additionally and increase research power by creating inter-departmental research themes that harness complementarity and strengths to address grand challenges of scientific and societal importance.

b. Congruence with university-level goals

The department contributes significantly by delivering excellent research, teaching, international profile and impact (research, societal, industrial) that is commensurate with KTH's position at Sweden's largest technical university. Sustainability goals are embedded in the departmental strategy and outputs. International collaborations contribute significantly to research outputs.

It is noted that the university goal and strategy on Digitalisation is unclear since this broad heading encompasses many aspects, so it is difficult for departments to align appropriately here.

c. Leadership structure and collegial structure

The department is divided into four divisions, each with a divisional head. The Head of Department liaises between the school and the department. There is clear evidence that the department is run very well with real leadership and a high degree of collegiality, inclusivity, consultation, mentorship and support. This aspect was very impressive and delivers a high functioning department and engenders a positive and welcoming working environment for researchers and staff at all levels. It is a key factor in retaining high morale, motivation and institutional loyalty. Young faculty can operate with research independence within a supportive and collaborative environment that allows talent to be nurtured and developed.

It is noted that two divisions are geographically separated in other sites, so strategies to facilitate networking, joint seminars, etc. need to be developed and supported by the School.

d. Strategies for achieving high quality

The departmental culture provides an excellent environment for delivering high quality, with access to collaboration, infrastructure, collegiate support and annual development dialogues. This is demonstrated in high impact publications and leadership in important areas of research. High quality research supervision is provided to PhDs and postdoctoral staff.

The department has, thus far, been successful in attracting external research funding, international and industrial collaborations and delivering high quality outputs. However, continuing success will depend critically on attracting further external funding and also on a significantly improved funding settlement from the School. The current financial and administrative burdens placed on staff need to be alleviated in order to sustain research at the highest level.

There is a real opportunity to consolidate the departmental and inter-departmental research strengths in order to address specific grand challenges with the critical mass and research power required to create a unique leadership position for KTH.

4. Interaction between research and teaching

a. Interaction between research and teaching at all three levels (B.Sc., M.Sc., Ph.D.) of education

The Department of chemistry carries the largest teaching burden in the School, with all academic staff involved in delivering several degree (3y BSc + 2y MSc) programs (Biotechnology, Energy and Environment, Material Engineering) and Engineering Chemistry. Masters programmes include Molecular science and engineering; Chemical engineering for energy and environment; Macromolecular materials; Industrial and Environmental Biotechnology; and, Medical biotechnology. Sustainability is an important thread running through teaching and research and this aspect is particularly attractive to students.

There is a direct and positive connection between research and teaching at all levels, exposing students to state-of-the art knowledge in specialist areas. This integration between research and teaching is commendable and underpins the department's success in producing graduates that are highly prized and sought after by industry. Postgraduates are also involved in supervising undergraduate research projects and as laboratory assistants, thus embedding a grassroots scholarship culture. However, the reduction on PhD students, arising from the substantially increased costs, will impact on this in the future. Loss of PhD numbers will also increase staff teaching loads, affecting research time.

PhD courses are available with PhD students undertaking 60 credits worth of modules. However, a lack of funding is impacting on the diversity of PhD training available. Most PhDs are completed within a 4-4.5 year span.

5. Impact and engagement in society

a. Relevance, scale, and impact of the department's current engagement with society and industry

The department has created high impact with society and industry in a number of areas. First and foremost, it creates skilled graduates and PhDs who are highly prized by industry. There are also close ties between individual researchers and 100+ industries, with a number of sponsored PhDs, collaborative projects and contract work, thus translating academic knowledge into the technological sphere. Some faculty staff also hold part-time positions in companies.

The exemplar impact cases provided in the self-evaluation were impressive.

Departmental research has led to spin-out companies, e.g., the creation of the company Dyenamo AB, which produces and sells chemicals and instruments testing and development of dye-sensitized and perovskite solar cells.

b. Research dissemination beyond academia

The department participates actively in national outreach events such as "Forskarfredag", and targeted outreach in local schools, and contributes leading roles in the Swedish Chemical Society, which facilitates societal influence and national dissemination.

c. Relation to sustainability and the United Nations' Sustainable Development Goals (SDGs)

The department's research maps directly onto the United Nations SDGs, with 50-60% of research related to sustainable development. All new faculty positions are also associated with at least one SDG. Sustainability is also present in the teaching. Overall, this alignment with SDGs and clear signposting of sustainability and societal challenges is attractive for both undergraduate and PhD students.

d. Plans and structure for increased impact

The impact is largely driven at the grass-roots level within departments, often via one-to-one contacts between academics and external companies or stakeholders. Overall, the integrated impact is high.

However, there are no formal mechanisms or platforms to actively channel and organise industrial contacts and engagement e.g., as currently exist in TreeSearch or those utilised previously by the department via research institutes such as YKI and Innventia. The new 2MILab is developing an outreach plan for stimulating industrial researchers to work at KTH premises, using a full cost model.

At School level, there is an "impact responsible" person whose role is restricted to encouraging researchers to consider impact. Impact cases can also be promoted at School/Central level for fundraising activities. However, there appears to be no effective institutional framework or direct resource to capture the breadth and depth of this impact, or indeed to reward it (e.g., via salary contribution). However, large and prestigious collaborations/start-ups do accrue credit from School and the University and are a factor for promotion.

Legal support is provided by KTH with a recently established single administrative entry point at School level to coordinate such actions. KTH Innovation is highly regarded and supports academics to develop patents and business plans, and also grants seed funds (typical size, 50-200 kSEK) for developing business ideas. Via KTH Holding AB, they also support researchers grants and guaranteed loans to cover costs associated with filing and maintaining patents. However, significant conflicts of interest have to be managed with university start-ups, which are encouraged to locate on campus and use departmental equipment and expertise, and requires clear delineation between activities done by the start-up (private organisation) and those done at KTH (state organisation).

6. Recommendations for strengthening the department and its future potential

There is a real opportunity to consolidate the departmental and inter-departmental research strengths into cross-cutting inter-departmental themes in order to address specific grand challenges with the critical mass and research power required to create a unique leadership position for KTH. The panel noted potential inter-departmental connectivity in solar energy, electrification, catalysis, clean sustainable materials, surface corrosion and tribology, bio-based materials, and connecting nano level measurements to processes and performance in the real world. However, academic staff will need time and space to explore and implement this and this process needs to be supported by the institution.

Advanced science needs increasingly advanced instrumentation to remain competitive. A longer term infrastructure plan is recommended. KTH will have to consider how more permanent technical support can be provided at the departmental level to support this infrastructure.

The current KTH financial model needs to be revised in order to safeguard departmental viability and provide the space and time for faculty to strategize, develop, and sustain future research initiatives at the highest level. The current model is also adversely affecting recruitment and retention of talent.

Recruitment plans to replace expected academic retirements need to be implemented so that new faculty are accommodated without loss of momentum. Competitive starting packages and financial frameworks will be critical to attracting talents to KTH. The current ability of young faculty to operate with research independence within a supportive and collaborative environment needs to be retained and protected.

KTH administrative culture and frameworks need to pivot towards alleviating academic workload, be more agile and efficient (e.g., in recruitment), be made available locally at the departmental level and be responsive and open to academic needs and strategy.

Impact activities should be recognised and rewarded by KTH (e.g., via salary contribution).

The department's impressive internal leadership and collegiate culture is a key asset and needs to be supported and safeguarded to ensure a high functioning department.

It is noted that two divisions are geographically separated in other sites, so strategies to facilitate networking, joint seminars, etc. need to be developed and supported by the School.

7. Final remarks

The panel was provided with a clear and honest self-evaluation document. The discussion with the department included a short and informative presentation by the department, followed by questions from the panel. The discussion between the panel and departmental representatives was open, articulate, relevant to the RAE and honest. In addition, a short 15 min discussion was held between the panel and young researchers (PhD, researchers, assistant professors), which was also open and honest. The clear message received from this group was that they genuinely enjoyed working in the department and found the environment supportive and stimulating.

Overall, this is a strong and vibrant department with a leading research and teaching profile and an excellent departmental culture. There are real opportunities to consolidate and strengthen its research and impact in the future via strategic, synergistic alliances within KTH and formulating cross-cutting themes.

However, the department is at a critical point regarding internal KTH funding and central administration and recruitment frameworks, which needs to be addressed by both the institution and the KTH central administration.

Department of Chemical Engineering

Major findings

1. Strengths and weaknesses of the department

Concerned and recommendations for improvement

The department counts 4 divisions, covering diverse aspects of chemical engineering. They are different in size and some are identified as possibly subcritical by the department.

Main strengths identified are: subject areas are related to the KTH pillar sustainability and contribute to solving challenges of the society, high level scientific output, important external funding, both fundamental and applied research are done and this in strong cross-disciplinary collaboration in academia and industry, local access to infrastructure, up-to date equipment, advanced characterization instruments, and proximity of the divisions. Numerous collaborations with Swedish companies are a major strength of the department. They are often developed in large projects along with other academic partners, promoting thereby multidisciplinary research. The department is a key, sometimes founding, partner in several major research Swedish centres on Gasification, Electromobility and Energy. This involvement in research centres is clearly a strength of the department.

Main weaknesses identified by the department are: limited visibility as a department outside, potential of collaborations within the department not fully utilized, insufficient internal funding and as a consequence lack of funding for method development, no strategy to obtain prestigious funding, slow employment process, too high administrative burden. The limited visibility is due to deficient communication.

Vision and opportunities to strengthen the research are driven by keeping the balance between fundamental and applied research and this has a strong impact on the recruitment of new assistant professors. The department has a long term strategy, in particular related to the sustainability goal, but the implementation of this long term strategy is difficult because of fluctuating external funding and of the unknown future societal needs.

Threats and risks are strongly related to the dependence on external funding. The effort to obtain those goes at the expense of optimising collaborations in the department or in the school.

2. Relevant and forward-looking objectives

Are the goals relevant and forward-oriented?

The department aims to become an international leader in using chemical processes for decarbonization of the society, including electromobility, circular processes and decarbonization of industry. It clearly has the potential to achieve this ambitious objective considering its excellence in research and unique facilities. A more detailed roadmap to reach that goal is under construction for more than 1 year. Where the focus will be will depend on the requirements from the society and the availability of external funding. When looking at the future, the department needs to keep in mind that currently, as stated in the SER, the largest part of the external funding comes from the Swedish Energy Agency, meaning that it is critical for the department.

The goals are relevant and forward-oriented in the short term. But in the long term the situation is less clear. Note that the construction of the road map has unfortunately been impended by the pandemic.

3. International community engagement

The department is involved in international collaborations, but the position in EU projects is mostly at the level of participation (collaborative or training oriented (ITN)), due to lack of time to take up the coordination. The support from KTH is at the level of administration and much less on how to write a proposal that has high chance to be approved.

4. Future potential of the department

For a positive development towards fulfilling their goals, operating on the front line of international research, and exerting a beneficial impact on society

With the long term topic of decarbonization, the department has the potential to exert beneficial impact on society and can clearly be at the frontline of international research. To reach that goal, choices will have to be made, as well at the level of topics as at the level of organisation within the department. The roadmap needs to be written and implemented.

5. Recommendations

Based on your overall observations and analysis of the department, please provide the recommendations that you find most useful to the department for the future development of high-quality research and research environments

The top priority for the department is to work out the roadmap towards a leadership position in decarbonization. The strategy defined by the department would benefit from shorter recruitment procedures. To achieve and maintain the pursued position, the balance between seed money and external funding should improve. The visibility as a department could be improved with more efforts in communication and possibly with support from communication services of KTH. It seems that there is also a problem of overlap with other departments. This clearly makes the visibility more difficult. Some topics are closely related to research at the Chemistry department or at the Materials Science and Engineering department (batteries, electrode materials, structural batteries as examples). These topics are investigated with distinct perspectives, expertise and facilities. This situation provides an opportunity for establishing world leading multidisciplinary task forces at KTH in these fields. Collaborations are already existing, but they would benefit from more visibility in a more coherent way by crosscutting teams sharing common interests (see general comments).

Specific issues

1. Research profile and quality

a. Central research questions and themes, and main research activities

At this point, there is a rather large diversity in the research questions addressed by the different divisions and this both at the level of topics and at the level of approaches. Topics: several aspects of energy devices and processes are covered, together with resource recovery. Approaches: from researching new materials for energy devices to more fundamental thermodynamic studies of processes. This makes it difficult to identify the research profile of the department. The unique selling point identified by the department is collaboration with industry solving relevant questions for sustainability. This is a very broad basis to translate in a clear profile.

The quality of the research is excellent and at the highest international level, as illustrated by the research output in terms of publications, the high success rate in attracting external funding, and successful innovation achievements.

b. Contributions to the advancement of state of the art within the research fields of the department

The department has successfully contributed to the advancement of state of the art in its research fields, in particular regarding electrochemistry, electrode materials, gasification, ageing of catalysts and batteries, resource recovery systems, sensing technologies, and steel industry. The department takes orientations in cutting edge-research fields concerning in particular implementation of biotechnologies in materials science, use of life cycle assessments, artificial intelligence and machine learning in future projects. These directions appear to be particularly relevant and appropriate to remain at the forefront of research in the broad fields of sustainability, energy and environment.

c. Quality and quantity of contributions to the body of scientific knowledge, engagement in national and international research collaboration within academia and its outcomes

The department is particularly strong in attracting external funding, especially from industry but also in international collaborations. Doing research in the context of industrial funding does not jeopardize the scientific output. It seems that the department is exceptionally strong in its engagement in national research (key partner, coordinator of national research centres) but less at the international level.

d. Follow-up from previous evaluations

According to the SER, the main recommendation of RAE2012 was to reinforce basic research. As follow-up, many large projects have been initiated with researchers of other departments at KTH and other universities. From the discussion, we learn that it is always a trade-off between internal knowledge built-up and collaboration due to lack of time. A good example of follow-up in house is the recent recruitment in the field of modelling.

2. Viability and research environment

a. Internal and external funding; current status and strategies for the future

The department depends strongly on external funding. This is positive on its own, but leads to the formulation by the departments of an important weaknesses: ‘We need to follow research agendas set by others’ and ‘Funding opportunities are often focussed on applications and not on method development’. The department tries to remediate by recruiting new research profiles, but is hindered by the slow recruitment procedures and the harsh requirement for faculty members to provide part of their salary from the external funding.

The department is heavily involved in several Swedish centres (Swedish Gasification Centre, Swedish Electromobility Centre, Battery Sweden, StandUp for Energy, Swedish Knowledge Centre for Renewable Fuels (f3), SwedNess, Wallenberg Wood Science Centre, and PUSH, i.e. Production, use and storage of hydrogen for sustainable energy systems) and the European initiative Fuel Cells and Hydrogen Joint Undertaken. This is, according to the department, a major source for funding and coherence in research strategy. It has therefore to be encouraged and pursued.

b. Academic culture

The academic culture is based on interaction between professors and researchers and discussions at department level through lectures, planning meetings, department meetings, teacher teams. The idea behind it is that if people know each other and their activities, this will open up for collaboration across divisional boundaries. The teaching load is distributed over the different professors in the department.

c. Current faculty situation and composition of the research team(s)

There is a strong concern about the number of PhD's that can be recruited. They cannot be financed by scholarships anymore and this increases the cost and as a consequence lowers their number. This has an impact on the amount of research that can be performed. Recruitment of new assistant and associate professors is essential for the future of the department, and this is identified as a very slow process, with strict boundary conditions. As a result, some applicants refuse the job, and others leave the department early.

The recruitment of young researchers in the department appears to be critical when one considers the age distribution of professors, several next retirements, and the ambition of the department to tackle new scientific directions, needing the input of new expertise.

d. Recruitment strategies

See above.

e. Infrastructure and facilities

The fact that the department is gathered in one building is considered as advantageous and facilitating access to advanced instrumentation. The department has the ambition to extend its own arsenal of techniques and to contribute to the development of the school's system for joint instrumentation (2MILab). Bottlenecks are: allocation of money on projects to that purpose with a long decision line as a consequence, no permanent technical staff for the operation and maintenance of the equipment, no clear procedures to obtain measurement time.

3. Strategies and organisation

a. Goals for development 5–10 years ahead

The vision of the department is that research and education need to address the challenges of today and tomorrow, with special emphasis on energy and environment. Students are educated according to high international standards, with special attention to innovation.

The ultimate goal is to be leader in Sweden on research and education regarding the use of chemical processes for decarbonization of the society.

Main action points are: recruitment of well-balanced faculty considering gender, background and competences; strengthen basic funding of faculty to become less dependent on external funding; reinforce collaborations inside and outside the department.

To reach these goals, the department must continue to construct its roadmap and follow its long-term strategy.

b. Congruence with university-level goals

The four pillars for KTH are: sustainability, equality, digitalization, internationalization. The department has a clear view on how to contribute to sustainability, equality and internationalization. The strategy to contribute to digitalization is in a starting up phase: the team working on gasification is familiar with big data handling but in general introduction of techniques of artificial intelligence and machine learning seems to be in a premature phase. There is no clear procedure for data management at department level.

c. Leadership structure and collegial structure

The division is organised in four divisions. The head and vice-head of the department together with the 4 heads of division form the management group. Interaction with the department and divisions goes through regular meetings where issues related to teaching, research, staff, economy are discussed. Important task in the near future is the discussion of the roadmap. It is essential for the divisions and the department that consensus is reached on how to evolve the coming years.

d. Strategies for achieving high quality

PhDs take a crucial position in performing research. The department has a strategy in place for guidance, supervision and creating output involving postdocs, assistant professors, associate professors and professors. High quality research is performed. The declining number of PhD students is a negative evolution that needs to be stopped.

4. Interaction between research and teaching

a. Interaction between research and teaching at all three levels (B.Sc., M.Sc., Ph.D.) of education

The interaction between research and teaching is strong. The close research cooperation with industry is reflected in teaching making it societal-relevant. At bachelor level it is reflected in research assignments with industrial relevance. Master diploma work is often performed in an industrial lab. At PhD level, the teaching is very strongly related to research.

The consequence is that graduated master students often prefer to go to industry instead of going for a PhD.

The proportion between time spent in research versus teaching is estimated to be 75/25%. On top of that comes an administrative load imposed by KTH regulations that is becoming heavier and heavier.

5. Impact and engagement in society

a. Relevance, scale, and impact of the department's current engagement with society and industry

All the divisions of the Chemical Engineering department work on relevant issues with significant societal and industrial impacts. The main topics include research on decarbonisation of steel industry, cleaner chemical processes, electrification of the transport sector and gasification of biomass. The current engagement in this field is manifested by strong and numerous collaborations with industrial partners and by substantial funding from the Swedish Energy Agency. The engagement with society and industry is clearly a strength of the department.

b. Research dissemination beyond academia

According to examples provided by the department, several faculty members are convincingly active at communicating research to the general public. These examples include prestigious visits by politicians, interviews in newspapers, radio and television programs. This point can therefore be also considered as a strength of the department. Nevertheless, it would also be important to not forget communication towards young people. This could perhaps be organized through presentations in secondary and high schools, and outreach activities within the laboratories for schools, and families.

c. Relation to sustainability and the United Nations' Sustainable Development Goals (SDGs)

As indicated above, the research of the department falls within the broad field of sustainability with most of the topics directly related to energy and environment. Almost all publications of the department are thereby related to SDGs (in particular SDG 7, SDG 13 and SDG 12).

d. Plans and structure for increased impact

The department demonstrates a great ability to direct its research towards high impact topics using the most innovative approaches. The department was able to carry out strategic recruitments in the last years to remain at the highest international level. However, this ability does not seem to be based on a particular structuring of the department, nor on the establishing of a long-term strategy for increased impact. The department appears to be aware of this deficiency and indicates its work establish a roadmap. This is an excellent initiative, which remains to be pursued and implemented. Increasing the impact of the department may also involve a strategy at the level of other departments Collaborations are existing and fruitful. But, it could be useful to develop crosscutting teams on subjects of common interest in the different departments (batteries, cellulose, steel), in particular for more visibility at the national and international levels.

6. Recommendations for strengthening the department and its future potential

As indicated above, the department of Chemical Engineering performs exceptionally well in its research. It enjoys a good balance of experimental and theoretical work, as well as a good balance of applied research and application driven basic research. The excellence of the department is manifested by numerous publications in high impact journals, an exceptional efficiency at attracting external funding and at developing collaborations in the industrial and academic worlds nationally and internationally. The department provides an excellent environment for young researchers and students, who can benefit from regular support from the older faculties but also from freedom to develop themselves. Last, the department enjoys state of the art facilities for the synthesis and characterizations of materials in addition to unique home-made engineering tools.

However, in spite of these strengths and outstanding performances, the department activities and future potential could be improved at different levels.

As indicated above, it seems that the department suffers from difficulties to implement its long term strategy. Future directions are expected to depend on external fundings and future societal needs. This can be somehow understood considering the pressure on external funding, and the insufficient internal funding. In spite of these difficulties, the department has identified the need to establish a road map for future activities. This initiative appears to be particularly relevant.

The department has shown its ability at choosing new and relevant directions. Development of these new directions calls critically for the recruitment of young researchers. This need appears even more critical when one considers the distribution ages in the department and the future retirements.

The choice of new directions is clearly a strength, but the department should also strengthen collaborations at the local level without spreading too much. In particular, it seems that more collaborations between experimentalists and theorists could be useful among the different departments of the schools of Engineering Science in Chemistry, Biotechnology and Health and of Industrial Engineering and Management.

Several topics relevant in the broad frame of sustainability are investigated in different departments of the above schools. This is an opportunity for creating world-leading task forces in these fields with distinct expertise and facilities.

Based on the existing collaborations and future ones, it could be useful to develop crosscutting teams to gather the research efforts on well-defined topics (examples electrode materials, structural batteries, cellulose, steel, solar cells). That could increase impact and visibility of the research, in addition to provide openings for new progresses through interdisciplinary work.

The department enjoys a number of collaborations at the international level in various fields. It is also involved in several international projects and networks. The department is most often acting as a partner in these projects. More leadership could perhaps be achieved with the coordination of large EU projects. Of course, this has to be done in realistic conditions, providing sufficient support from KTH for preparation of the proposal and administration of the projects. The same holds actually for prestigious research funding.

7. Final remarks

In addition, state if the panel lacked any material relevant to making adequate observations and recommendations.

The panel has regretted to not physically meet the department members, and to not visit the infrastructures. This could have facilitated scientific discussions on research activities, and a better appreciation of the unique experimental facilities available.

In addition, the panel had difficulties for evaluation because of lack of information on relationships between the departments and the schools and the central KTH administration. It was not clear for the panel how strategic decisions at KTH are taken and discussed with the departments.

Department of Materials Science and Engineering

Major findings

1. Strengths and weaknesses of the department

The department is relatively large and consists of three unit that cover several aspects of the backbone of materials science and engineering: processes, structures and properties. The 4th essential part of MSE "performance" is largely established by collaboration with other departments and/or with industry. The self-evaluation identifies strengths and weaknesses in research and organization. Opportunities and threats are not explicitly formulated in a SWOT analysis.

Research wise, MSE has certainly been world leading in several topics for many years, not at least in thermodynamic and quantum mechanical modelling activities of relevance for real materials (not just benchmark cases) and they are among the first movers in integrated computational materials engineering (ICME). They have an extensive international academic and industrial network in metals and cemented carbides related research. Their track record in external funding, involving industry is very strong and most relevant for their application-driven fundamental research approach.

The department is to a high degree multidisciplinary, and combines disciplines in physics, chemistry, manufacturing engineering and metallurgy; bridges across length scales from electronic level to the macro level of steel production and combines computational and experimental research. This unique combination of expertise makes MSE a most attractive research partner. At the same time, it could also be difficult for potential external collaborators to see where the focus is. On the other side, the internal dialogue between these different disciplines, who speak different scientific languages, can be challenging, but is also enriching for the department members. As identified in the self-evaluation, MSE has not been able to exploit their full potential in the process-structure-properties(-performance) space. An obvious example is that neither the report nor the department's website highlights an important driver in basic and applied research of additive manufacturing of metallic materials. On paper, MSE would be excellently equipped with know-how, experimental and computational resources to contribute importantly to this hot topic, actually they would be the best in academic Sweden to contribute. From the interview we learned that several projects are (about to be) initiated and are carefully planned. This appears to come rather late, as KTH-MSE has no visibility (yet) in this rapidly developing topic.

The subdivision in 3 units appears a logical one, but may also hinder common activities across the units. Since the report was written, a slight change in the organizational structure has been implemented to mitigate this, by coordinating computational activities across the 3 units. Experimental activities across the 3 units all rely on the Hultgren laboratory. There is a positive working atmosphere, despite imbalance in the work-load distribution among the faculty and the researchers.

The department appears attractive for students and young researchers. A clearly visible contribution to a sustainable society and circular economy are the attractors, as well as the good possibilities in Swedish industry.

2. Relevant and forward-looking objectives

The ambition of MSE is to become a world-leading department of application driven fundamental research of metallic and ceramic materials. Contributing to a sustainable society is very high on the agenda and is an important driver for external funding of research.

3. International community engagement

MSE is an important, highly esteemed and well-known international player in many aspects of “hard” materials research and they have a long-standing tradition for this. The thermodynamic and kinetic modelling software from their spin-out Thermo-Calc, established in 1997 (but with a much longer history), is used in 60 countries and by 1300 organizations for innovative materials design; this was a most visionary development and has been an important driver for the current ICME movement and computational materials design. MSE has high international visibility in academia and plays a leading role in computational thermodynamics and quantum mechanics of real materials (metals and cemented carbides), in phase transformations in materials and in green-steel production. They collaborate with excellent universities around the world and recruit their PhDs from the best universities; their most important “product”, i.e., their PhDs, are highly appreciated around the world.

4. Future potential of the department

Currently, the research portfolio relies heavily on the Swedish steel producing and steel applying industry. Although this industry is still strong in Sweden, on a global scale steel production is more and more concentrated in Asia, driven by lower production costs and (so far) less restrictive environmental issues. The department has the academic competences and potential to enter into many fields of materials science and engineering, in particular as a first mover. They just have to decide where they want to go. Nevertheless, they do not appear to be as agile as the sum of their competences should allow them to be. There can be various reasons for this, not at least the strong dependence and continuous focus on acquiring external scientific and industrial financing and insufficient freely applicable financial resources for curiosity-driven research. This is further weakened by tying up basic research finances to co-financing of underfinanced external research projects, not at least caused by a high internal overhead. Certainly, this is not a viable way to go and sooner or later a tipping point is reached. Another reason that may hinder agility is that the topics for external financing are perhaps too much defined by political winds and industrial needs. Another reason could be internal communication: are all the many different disciplines on the same page and do they want to focus on the same topics? It requires visionary and innovative PIs who can look far beyond their own research interests to bring the enormous potential into play. Employing highly talented assistant professors and give them freedom is a way to go; currently, there are very few assistant professors employed in the department. Last, but not least, rewarding granted major proposals with additional administrative tasks and long lead times for recruitment are counterproductive for an agile research environment at the forefront of international research.

5. Recommendations

MSE is recommended to define research targets that combine the available competences, are curiosity driven and less dictated by political and/or industrial needs. The vehicle is improved internal communication and recruitment of more talent at the assistant professor level.

Specific issues

1. Research profile and quality

a. Central research questions and themes, and main research activities

MSE research focuses on sustainability like CO2 neutral steel production, high strength steels, materials design via modelling tools and printed solar cells and batteries. ICME, Integrated Computational Materials Engineering, thermodynamic and kinetic modelling software are central research areas where MSE plays an important and world-leading role.

MSE's strategy is to enter research areas where they have a unique competence to add. As an example, the entrance into Additive Manufacturing was well-planned and based on the gaps identified for powder processing and powder material suitable for AM technology. The competences united within MSE in principle would allow them to be an important game-changer in this rapidly developing field.

b. Contributions to the advancement of state of the art within the research fields of the department

These are very well described in the self-evaluation report and not repeated here. MSE has a long-standing reputation to be among the world leaders in physical metallurgy, particularly in steels and computational materials design. MSE strengths and contributions are to a large extent in their uniqueness covering everything from process, structure, properties to performance; across length scales from electronic level to the macro level of steel production and combined with computational and experimental research. The strategy to focus on application driven fundamental research allows MSE to be in the forefront and contribute to a sustainable society, clean steel, and circular economy.

c. Quality and quantity of contributions to the body of scientific knowledge, engagement in national and international research collaboration within academia and its outcomes

During 2012-2019 MSE contributed with 1570 peer-reviewed articles (WoS) and 132 doctoral theses. MSE manages 2-3 national centres; CeXS, Hero-m 2i and MMD in which academia and industry are well represented. CeXS also manages the Swedish beamline at PETRA III at DESY, Hamburg. MSE also have two KTH infrastructure labs: Hultgren Laboratory and Modelling Laboratory. MSE also participates and coordinates national and EU funded projects, collaborating with partners in steel, energy, and mobility segments.

d. Follow-up from previous evaluations

Previous evaluations included recommendations on critical recruitment, collaboration opportunities with units in Chemistry and data management. MSE has realized parts of the recommendations for instance established collaboration on different levels and projects with departments within the CBH school. Data management procedures on group level has been realized on group level and is further explored to be on a more general level supporting efficient data driven research. The critical replacement recruitment of a new professor in solidification was unsuccessful and an interim solution was implemented. To avoid this situation in the future a recruitment strategy to identify need to replace a position eight years before retirement has been introduced.

2. Viability and research environment

a. Internal and external funding; current status and strategies for the future

MSE is very dependent on external financing and have been very successful on receiving both national and EU grants. This also makes MSE vulnerable to political, industrial, and societal turns to keep a long-term plan but the strategy to work with "fundamental driven applied research" is a smart way to mitigate this. External funding erodes the finances allocated through government grants, because co-financing is required and overhead on external funds is insufficient to compensate for the high internal overhead at KTH. This is not a sustainable development and it jeopardizes MSEs agility in pursuing curiosity-driven research.

b. Academic culture

MSE provides an open and including atmosphere, which is found in the possibility to approach supervisors and professors directly with questions and support, also outside the own research group. Students are proud of being a part of the department and compliment the quality of the lectures. Professor Malin Selleby was awarded as best lecturer by the students, which was highlighted by the students during the session.

c. Current faculty situation and composition of the research team(s)

The faculty encompasses 100 members of which 26 are women and 74 men. The faculty is divided into the three units Processes, Structures and Properties.

- Unit of Processes encompasses; 1 Professor, 3 Affiliated Professors, 4 Associate professors, 1 Assistant Professor, 5 Senior Researchers and 1 Affiliated Faculty
- Unit of Structure encompasses; 6 Professors, 1 Associate Professor, 7 Senior Researchers, 1 Affiliated Faculty and 1 Adjunct Professors
- Unit of Properties encompasses; 3 Professors, 2 Associate Professors and 8 Senior Researchers.

In particular, the number of assistant professors is critically low and needs serious attention to enter into new fields of research.

d. Recruitment strategies

Recruitment is based on both teaching and research needs. Female recruitments are difficult, and a better gender balance is aimed for. Now MSE have no faculty gaps but are in the process to map individuals' competences and skills to identify potential future gaps and to share faculty assignments more fairly. Technical support and maintenance of the equipment are to a large extent within PhD student's responsibility, which is not considered a sustainable long-term solution. Dedicated technicians are available for the more advanced and expensive instruments but need to be further improved.

MSE has a strategic approach to choose the level, for example Professor or Assistant Professor, to recruit attracted different competences. Assistant Professor positions generally attract more applicants with a broader palette of competence since it gives some freedom to tailor the area of interest.

Recent recruitment has been both successful and unsuccessful. Unsuccessful recruitment is explained by the difficulties to be competitive with other universities with more attractive economic and funding conditions. However, benefits like research freedom, personnel carrier development trainings and parental leave possibilities also play an important part.

e. Infrastructure and facilities

MSE is located in one building and with close access to all their equipment. MSE has a good range of advanced equipment, ranging from material processing to property evaluations and performance. Equipment is also accessible through collaboration with academic and industrial partners. The Hultgren laboratory is a part of KTH infrastructure, including equipment with a utilization of about 50%. The aim is to gather all equipment owned by MSE divisions under the umbrella of the Hultgren laboratory to facilitate and encourage open access via a future booking system.

3. Strategies and organisation

a. Goals for development 5–10 years ahead

The vision for MSE is: In 2030, MSE is a well-recognized as a world-leading department of application driven fundamental research on metallic and ceramic materials. In many areas MSE is already a world-leading department, not at least within the thermodynamic and kinetic modelling software and ICME. Improved collaboration on synergies within MSE is seen as a key improvement area both for the outcome of the department, but also to attract young researchers and research funds. Fundamental and applied research are integrated which makes the balance/ imbalance of less importance.

b. Congruence with university-level goals

MSE is well in line with KTH development plan and has clearly identifiable contributions to the four pillars “sustainability”, “diversity, gender balance and equal opportunities”, “internationalization” and “digitalisation”.

c. Leadership structure and collegial structure

MSE show a strong leadership structure with competent and approachable staff in leading positions. The set-up of divisions, competence centres and infrastructure labs; the structure and leadership are close to a matrix organization, which put a high working load for the leading staff. Some administrative support from the schools’ controller is highly appreciated but is limited to economy. The administrative requirement and workload have heavily increased the recent years and is considered to be a work environment issue, despite the efforts to balance the tasks among the faculty members.

d. Strategies for achieving high quality

MSE has a highly esteemed profile on delivering high quality research. An important output is master and PhD students that are attractive employees for academia and industry. PhDs take part in projects with a strong link to societal and industrial challenges, which leads to leading research positions in industry or an academic career within or outside Sweden.

Collaboration plan, communication plan, roadmaps of research areas and competences have been kicked-off to ensure high quality in different aspects. However, priorities and administrative assignments hinders the MSE staff to find time for discussions, finalizing and commit on these plans and roadmaps.

4. Interaction between research and teaching

The faculty and PhDs are involved in teaching and supervision on all 3 levels. Teaching is research-based, which is a motivating factor for the students. PhDs are involved in tutorials and exercises; they appear to be an important and vital resource in this respect.

5. Impact and engagement in society

a. Relevance, scale, and impact of the department's current engagement with society and industry

MSEs research activities are most relevant for the Swedish metallurgical industry, from steel producers to manufacturers of steel and cemented carbide-based applications. There is a strong collaboration with the major players in metallurgical Sweden. The most important impact is made by educating PhD students who are employed in academia and, particularly, in industry. Various software programs developed at MSE are used worldwide and are important tools in materials design.

b. Research dissemination beyond academia

Industrial partners are included in most of the larger project activities. Dissemination of research results beyond academia is through annual workshops with industrial partners, seminars, and symposia.

c. Relation to sustainability and the United Nations' Sustainable Development Goals (SDGs)

The department contributes to 10 of the 17 SDGs, as materials are crucial in many of the SDGs. Most notable are fossil free steel production, materials for magnetocaloric heat pumps and computational materials design rather than trial and error.

d. Plans and structure for increased impact

MSE works on developing a strategy to communicate results and how to increase their visibility.

6. Recommendations for strengthening the department and its future potential

More focus on curiosity-driven research to enable breakthroughs in scientific research. Breakthroughs in science and paradigm shifts cannot be planned by political agendas.

7. Final remarks

The panel lacks information on the boundary conditions for the departments in general. The supportive roles of the schools and central KTH administration are unclear. Departments need only a modest administrative toolbox for optimal functioning. It appears that the provided top-down administrative processes and procedures are over-dimensioned, self-sustaining, a goal rather than a tool and counterproductive rather than supportive for cutting-edge research. For the international panel members, the financing situation of KTHs research appears ineffective to perform internationally competitive state-of-the-art research and attract and keep international scientific talent. The faculty and researchers at KTH have our sympathy, because "it is hard to be a researcher" under the provided conditions. Nevertheless, the scientific achievements are impressive.

Department of Theoretical Chemistry and Biology

Major findings

1. Strengths and weaknesses of the department

The Department of Theoretical Chemistry and Biology (TCB) a unique research unit for theoretical and computational chemistry, because theoretical method and software development is combined with high-level state-of-the art applications at a balanced and equal level. This is rarely the case, and the review panel is not aware of any other place in Sweden, and usually the focus lies on only one of them. Despite its research breadth, the research team around Prof. Patrick Norman belongs to the World leading experts in quantum chemical software development for high-performance computing architectures and applications in the grand areas of energy and light-matter interactions. TCB as a whole as well as the individual members themselves are internationally well recognized and possess an excellent research output in terms of publications.

Despite its international visibility, TCB seems not well recognized within KTH. This comprises researchers at other divisions, e.g., Chemistry, Chemical Engineering, or Fibre and Polymer Technologies, despite their expressed need for further theoretical support, as well as the students at KTH, since practically no students join TCB for Bachelor or Master theses.

The largest weakness of the organizational structure of TCB is identified by the panel in the lack of local administrative support within the unit, and an extremely high burden of administrative tasks put on the professors by central KTH administration. This results in a lack of time for research, which will in the long-time put the success of TCB at risk.

2. Relevant and forward-looking objectives

TCB has a clear strategy how to further increase its scientific impact and how to pursue its scientific goals. It is planned to push the method development further forward to be in the best position to apply for larger national and European grants. Method development always puts a research unit into a unique, world-leading position, as it is a requirement to perform cutting-edge applications which are not yet possible with existing methods and computer programs. The taken measures to, for example, closely cooperate with the computer centre PDC are adequate and needed to achieve this goal.

The chosen areas of applications have convinced the panel, as they are highly relevant and future oriented. This still can be extended, parallel to the method development initiative, by reaching out into the other divisions. This is recommended by the panel, as this will increase the scientific strength of the school as a whole and open an avenue for collaborative research and larger funding possibilities. Natural collaboration partners are seen in the chemistry department, chemical engineering as well as in material science and engineering, where an interaction with the theory groups in particular can lead to fruitful cooperation.

3. International community engagement

TCB is highly international and internationally oriented. Its members are a broad international mixture at all levels: faculty, post-docs and doctoral students. For a long time, TCB acquired a lot of Chinese Science Council fellowships and hosted a large number of Chinese Ph.D. students due to their excellent scientific connections to China. TCB has fostered strong strategic international partnerships, which strengthen its research profile and visibility. TCB is active in European funding schemes, for example, the European Training Network on Computational Spectroscopy (COSINE), as well as in research

initiatives of the Nordic countries, e.g., NordCO2. Overall, TCB is already highly internationally engaged.

4. Future potential of the department

TCB has high potential to become a World leading research unit in the development of quantum chemical software for high-performance computing. After the initiation phase of the last four years, first programs have been devised and deployed to the international scientific community, which allow for the usage of highly parallel, state-of-the-art high-performance computing environments, which is not possible with the established program packages. This is a highly important and impactful endeavour, which is required for all computational science to adapt to the current paradigm change in hardware development away from faster individual CPUs towards large parallel and heterogeneous compute environments.

The chosen areas of application energy and light-matter interaction are highly challenging and timely, and they contribute to the fundamental understanding of the underlying processes paving the road to scientific breakthroughs and fundamentally new science and innovation. The accuracy of the theoretical predictions has become sufficient for them to be competitive with experiment. As a consequence, modelling and simulation can serve for predictions, guiding experimental work towards potentially successful efforts. This usually saves human as well as material resources, which should be stronger exploited between the divisions of KTH, by integrating TCB more strongly into ongoing research projects.

5. Recommendations

TCB is recommended to keep the 50/50 balance between theoretical method and software development and applications to state-of-the-art chemical and biochemical questions. This needs to be considered in upcoming recruitments.

The panel recommends TCB to become more strongly engaged in teaching undergraduate courses on quantum molecular sciences, theoretical and computational chemistry. Such courses should be part of any modern curriculum in chemistry, molecular biology, biophysics and material science. This will also boost research at TCB, since only through the promotion of the research activities of TCB at student levels access to talented and interested students can be achieved.

The division and the panel realises the weakness that success in acquiring external funding is unevenly distributed among the different members of TCB. Here the panel recommends to establish support measures internally within TCB by personal advice by experienced and successful individuals as well as externally by KTH, e.g. by financing courses in grant writing.

TCB is still not very visible at KTH and it is not scientifically anchored in research projects of other divisions despite their enormous need for theory support. The panel thus advises TCB to actively look for collaboration partners within KTH. This can for example be accomplished by organizing internal workshops or joint seminars. The new facilities of TCB may promote collaboration, but it seems unrealistic to believe that large numbers of collaborations just appear without actively looking for them.

Specific issues

1. Research profile and quality

a. Central research questions and themes, and main research activities

TCB pursues the development of highly efficient theoretical methods and corresponding computer programs for use on high-performance computing environments. In this context they developed the VeloxChem and Gator Program, which are modern modular computer programs easy to install and work with. They are made available as open-source programs.

In addition, the chosen areas of application are highly timely and innovative. Every single one addresses important questions in energy, light-matter interactions at a molecular level. TCB is one of the leading places for molecular response theory and computational spectroscopy in the World.

Practically all research at TCB is fundamental research, which very low applied aspects. Theory and method development is by definition fundamental, and these methods are applied within TCB to address, to the largest extent, fundamental questions in molecular sciences. This leads to a deep understanding of molecular mechanisms and structure-function relationships, which eventually paves the road to genuinely new ideas, impact and innovation.

b. Contributions to the advancement of state of the art within the research fields of the department

TCB is performing state-of-the-art research in all of its areas, which can be recognized at the high and extensive publication level of this rather small department.

c. Quality and quantity of contributions to the body of scientific knowledge, engagement in national and international research collaboration within academia and its outcomes

The established faculty members of TCB are internationally highly visible and contribute substantially to the advancement of the field of quantum molecular science, both in method development and application.

d. Follow-up from previous evaluations

TCB followed the recommendation of the previous RAE to establish a 50/50 balance between method development and application. In particular through the appointment of Prof. Patrick Norman, this has now been achieved, and a major initiative for method and software development has been established. By virtue of this effort, TCB has become a unique research unit in Sweden, which focusses both on development and theory.

The members of TCB did however not manage to integrate more strongly into the research areas of other divisions at KTH. This has been acknowledged in the self-evaluation already, and will be put in the focus for the coming years.

2. Viability and research environment

a. Internal and external funding; current status and strategies for the future

TCB relies heavily on external funding to cover the salaries of the faculty members and to continue their research activities. Due to the small portion of internal funds from KTH, the researchers at TCB do not have the flexibility to pursue high-risk projects or to provide proof-of-principle results for grant applications. Currently, they deal with this unfortunate situation by creatively using external funds for that purpose thereby putting the success of the funded projects at some risk. As soon as a major grant

application fails, the budget of the division as a whole is endangered, which will have severe consequences on the functionality of the department. This enormous risk puts a lot of pressure onto the faculty of TCB and thus generally hinders free and creative research in general.

The division as a whole follows the strategy to be internationally well connected and to pursue high-level method development to put them into the position to apply for large European grants together with their partner institutions. In addition, stronger scientific ties to other divisions of KTH are planned to be established to get access to interdisciplinary national funding resources.

b. Academic culture

The members of TCB have established an excellent academic culture. A high level of scientific exchange and collaboration within TCB and its members exists. In the panel discussion this high-level of personal interaction and open-mindedness became very clear. The panel members are impressed by the excellent atmosphere between the members of TCB.

c. Current faculty situation and composition of the research team(s)

At the moment the faculty situation is good and the size is sufficient to pursue the goals of TCB. With the recent recruitment of Nanna Holmgaard List at assistant professor level, TCB managed to broaden their research expertise towards nuclear dynamics and to hire the first female professor of the division. However, once Hans Ågren and Faris Gel'mukhanov retire, they will leave a knowledge and expertise gap behind that should be adequately closed with additional recruitments.

d. Recruitment strategies

The recruitment strategy at TCB largely relies on its excellent research atmosphere, both in terms of scientific excellence and international reputation as well as the friendliness and open-mindedness of its current members. Recruitment of the best talents, however, is generally hampered by the slow administrative process and the limited financial possibilities to quickly make competitive offers to high potential candidates. The possible offers are simply not competitive with the best European universities, a quality level that KTH is and should be aiming at.

e. Infrastructure and facilities

TCB moved into new facilities, which brings it closer to the other divisions of panel 3. This will naturally increase its visibility within KTH and thus facilitate scientific interactions. In addition, the required computational resources are provided by KTH and national facilities upon applications and appear to be sufficient for the research conducted at TCB. However, TCB wishes for more flexibility in usage of computer time, since it is limited to certain batches per month, which is often not sufficient at computational intensive periods of projects.

3. Strategies and organisation

a. Goals for development 5–10 years ahead

TCB plans to further foster its efforts in method development and to become a World leading place for quantum chemical method and software development in quantum molecular science for high-performance computing. It is also planned to keep an even balance between development of methods and their application to challenging questions in molecular sciences.

The members of TCB see the greatest challenges in the description of molecular systems attached to surfaces, which reaches into the fascinating areas of interfaces, surface science, and functional materials. The key problem is the lack of suitable theoretical methods and software. Here, TCB is a

unique position to on one hand develop the required methods and on the other to start going with addressing such problems.

The panel fully agrees with these goals, since this will secure the unique position in Sweden as a comprehensive theory unit in molecular science combining both high-level method development and state-of-the-art applications.

b. Congruence with university-level goals

The goals of the division are in line with the university-level goals, as the goals of TCB allow for reaching out into other scientific areas of the other divisions of KTH. This will lead to an overall strengthening of KTH as a whole.

c. Leadership structure and collegial structure

The leadership structure at TCB is excellent. Prof. Patrick Norman is a world-leading expert in theoretical chemistry with a clear vision for the future of TCB. Nevertheless, he manages to include all members of the division, faculty, postdocs and PhDs alike, in the decision making process. This leads to an exceptionally collegial atmosphere at TCB.

d. Strategies for achieving high quality

The quality of research at TCB is already at a very high level, which is documented by the high output of excellent publications despite the rather small size of TCB. Overall, the faculty at TCB pursues the strategy to supervise and train their Ph.D. students on a very high level thereby securing a high-level of research.

Continuous publication in high-ranked journals, as is pursued by TCB members is a key ingredient to ensure high-quality research.

4. Interaction between research and teaching

a. Interaction between research and teaching at all three levels (B.Sc., M.Sc., Ph.D.) of education

TCB suffers from the fact that it is not well represented within the curricula of undergraduate education. As a consequence, students are not aware of TCB and its research topics, and thus do not join for B.Sc. or M.Sc. theses. Therefore, it is equally difficult for TCB to recruit Ph.D. students from KTH, and as a consequence, they recruit largely internationally. International recruitment was for a long time supported by fellowships from outside of Sweden, e.g., the Chinese Science Council. Due to a policy change these fellowships are no longer possible at KTH, and as a consequence, TCB has lost many PhD students due to their exceptionally great connections to China. In the long run, this should be compensated by students originating from KTH.

For now the most important issue would thus be to integrate TCB into all curricula of the school, and thereby to give TCB access to students.

5. Impact and engagement in society

a. Relevance, scale, and impact of the department's current engagement with society and industry

Due to the nature of the basic research conducted at TCB, the current engagement with society and industry is rather scarce at TCB as outlined in the self-evaluation. The panel however is optimistic that this will increase naturally when more scientific collaborations with other research units at KTH arise, as it is planned by TCB and advised by the panel.

b. Research dissemination beyond academia

Dissemination beyond academia has just started as outlined in the self-evaluation. However, the members of TCB agreed to reconsider possibilities for outreach to society, and to pursue contacts to industrial partners more strongly.

c. Relation to sustainability and the United Nations' Sustainable Development Goals (SDGs)

The relations to sustainability are convincingly outlined in the self-evaluation report and are considered to be sufficient by the panel members.

d. Plans and structure for increased impact

For a theory department pursuing basic research on fundamental questions it is generally difficult to create or even increase impact. However, the panel recommends to consult other divisions at KTH for advice. Other options for increased visibility are to seek possibilities to communicate the research to the public in lectures and publications, or even via social media.

6. Recommendations for strengthening the department and its future potential

TCB is on an excellent path with a clear scientific strategy. The head and the members of TCB are well aware of the weaknesses and the potential of TCB and are constantly addressing them and working on their improvement.

For the near future, two aspects are pressing: 1) TCB needs to get access to undergraduate teaching and thus students, which is of prime importance for recruitment of well-trained Ph.D. students and gaining visibility at KTH. 2) TCB needs to actively seek for collaborations with scientist at other divisions to leverage the full potential of theory within the molecular sciences.

In general, the administrative workload of the professors needs to be drastically reduced to provide time and freedom to develop ideas and creativity to promote disruptive and innovative research. KTH needs to urgently find measures to support the professors at TCB and KTH in general to achieve this. Otherwise, the panel members see the existing high quality and breadth of research at TCB and KTH at risk.

7. Final remarks

To evaluate the performance of a division at KTH, the panel needs more information on the general administrative structure at KTH. Practically no information on the role of the schools at KTH is given, as well as on the decision-making processes at KTH. This includes the interaction points of researchers at the division with central KTH administration, and the measures taken by KTH to communicate with them, to get their input, learn their needs and to improve upon it.