## **Evaluation of Natural Sciences 2022-2024**

# Evaluation report Department of Chemistry University of Oslo

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## Statement from Evaluation Committee I

The members of this Evaluation Committee have evaluated the following administrative units at the higher education institutions within natural sciences in 2022-2023 and submitted a report for each administrative unit:

- Geophysical Institute, University of Bergen
- Department of Earth Sciences, University of Bergen
- Department of Physics and Technology, University of Bergen
- Department of Chemistry, University of Bergen
- Department of Theoretical Astrophysics, University of Oslo
- Department of Geosciences, University of Oslo
- Department of Physics, University of Oslo
- Department of Chemistry, University of Oslo

The members of the Evaluation Committee are in collective agreement with the assessments, conclusions and recommendations presented in this report. None of the Evaluation Committee members has declared any conflict of interest.

The Evaluation Committee has consisted of the following members:

Prof. James Kirchner (chair) ETH Zurich, Switzerland

Prof. Florencia Canelli University of Zurich, Switzerland Prof. Thors Hans Hansson University of Stockholm, Sweden

Prof. Isobel Hook

Prof. Gideon Henderson University of Oxford, United Kingdom

Prof. Nicola Hüsing University of Salzburg, Austria University of Lancaster, United Kingdom

Prof. Dieter Schinzer University of Magdeburg, Germany

## Description of the administrative unit

UiO KI researchers are organised in seven academic sections: Chemical Life Sciences, Electrochemistry, Catalysis, Theoretical Chemistry, Inorganic Materials Chemistry, Organic Chemistry, and Atmospheric Chemistry.

In 2021, KI (including its centres) had 198 employees, out of which 36 were professors or associate professors, seven lecturers, 40 post-doctoral researchers, 62 PhD scholars, 15 administrative staff and 38 technical staff.

In the self-assessment, KI emphasises its focus on supporting curiosity-driven research in chemistry, measuring its impact through international recognition, publication quality, and competitive grant success, aiming to contribute long-term insights, methods, and techniques to the field. The administrative unit collaborates with industry and research institutes, participating in programs like FME and SFI, to develop processes and products.

KI's self-assessment highlights several key points related to the connection between their work and their strategies. There is a recruitment plan (Fagstrategi) that involves reducing eight positions from 2022 to 2027. This negatively affects organic and physical chemistry, but safeguards sections like Theoretical Chemistry, Inorganic Materials Chemistry, Electrochemistry, and Catalysis, of which the latter three are affiliated with the Centre for Materials Science and Nanotechnology, SMN. The plan also includes renewed positions in Environmental Chemistry (Atmospheric Chemistry) and Soft Materials (Chemical Life Sciences).

KI is focused on acquiring advanced scientific equipment through external funding sources. They aim to balance resource distribution, supporting both active research groups and smaller promising research environments. They aim to address societal challenges while adapting to political constraints and changing funding priorities, all while maintaining research income.

KI's self-identified internal strengths include numerous research groups and a wide range of chemical expertise, along with valuable centres like Hylleraas, SMN, iCSI, and participation in FMEs, providing access to extensive resources. However, internal weaknesses encompass suboptimal funding for heavy experimental research, outdated infrastructure, and challenges in securing external funding, especially from RCN. They aim to balance cooperation within UiO while maintaining specialised research for teaching. Externally, KI sees opportunities in enhanced collaboration among research groups and sustainable development programs, including energy transformation. Anticipated developments like a new building and a focus on the Life science priority area are positive prospects. Increasing public visibility is also viewed as an opportunity. However, external threats involve declining government and RCN funding trends for basic research, potentially impacting the quality of research and education, and limiting their ability to redirect scientific efforts through new recruitments. Concerns also exist about potential political interference affecting autonomy and strategic decisions.

## **Overall assessment**

The overall assessment is based on the written material provided by different sources during the evaluation process, mainly the self-assessment of the administrative unit and the evaluations by the expert panels of the different sections of the administrative unit. The administrative unit is organised in seven sections (plus a didactic group), which one can find in a similar way in Chemistry Departments around the world. The organisation and management of the administrative unit is well thought through and combines research and teaching on a leadership level. These leaders of the different sections and teaching leadership meet on a regular time schedule to discuss the operation of the Department monthly, and they also focus on strategic issues. A more detailed view and considering the evaluation of Natural Sciences 2022-2023 provides a quite diverse picture of research performance within these sections.

Finally, the administrative unit provides three impact cases which deal with highly important topics that should strengthen the societal importance of the research, including outreach activities and possible business cases for important technology transfer in the area of climate change and new technologies for chemical industry.

#### Organic Chemistry (OrgChem)

This section provided a quite euphoric picture in its self-assessment stating to be one of the most productive and innovative sections in Norway and even abroad.

However, the Evaluation Committee believe that the facts and detailed analysis of the natural science evaluation show a different picture. Based on the large number of professors and PIs located in this section, the research performance is rather low – measured in the number of research publications and the amount of grant money brought in required to sustain high levels of research in the future. There is also a lack of innovative topics and almost no international or industrial collaborations are reported.

#### Inorganic Materials Chemistry (InorgChem)

This section is rather small and provided ambitious goals in its self-assessment becoming a leading group in Norway and at UiO in the areas of solid-state chemistry, inorganic materials chemistry, and nano chemistry. The group also report wanting to strengthen their existing expertise through the use of synchrotron and neutron large scale facilities. However, the ambitious goals are not realistic, based on the resources available. On the other hand, external funding is good, and the scientific output is very good from the group.

#### Catalysis (CatChem)

This section has an excellent track record; the group is active in important and up-to-date topics, is involved in many international collaborations, and has a very good strategy for knowledge transfer into applications. Heterogeneous and homogeneous catalysis are not well balanced in the section and most importantly, one of the key professors is close to retirement. It will be eminent to hire an international high-level scientist to fill this gap and to sustain the high performance of the section in the future.

#### Electrochemistry (ElChem)

This is also a strong section covering a wide range of topics, including solid-state electrochemistry, electrocatalysis, and photoelectrochemistry. The research performance is excellent, and the group is an international pioneer with the discovery of proton conduction in ceramic materials at elevated temperatures. The funding level is outstanding, and they show a very high level in published papers. In general, their research has high economic relevance. Again, the leading figure of the section will

retire quite soon and a clear plan to fill that appointment will be of great importance for the future success of the section.

#### Chemical Life Science (ChemBio)

This section is very large (60 scientists), and it is active in many important topics, including biomolecules, bioanalytics and biomaterials. The research section generates many high-level publications and high-level collaborations. The section has a clear vision, strong aims, and is internationally competitive with high standards.

Based on its large size, a new building is planned for 2026 which will also improve the internal collaboration of the research groups. Industrial collaboration could be improved to further increase the societal impact of the work.

#### Environmental Chemistry (AtmChem)

Although established in 2014, this section is rather small and depends very much on one professor who has also responsibilities at another university. The management of the section should be improved according to the Evaluation Committee, but the research output in terms of high-level publications is strong and a good level of funding is attracted.

The critical mass of the section should be increased to provide better career development for earlystage researchers. This task will be only successful if a better recruitment strategy is developed (see section 1.1).

#### Theoretical Chemistry (TheoChem)

This section is the largest theory group in Norway consisting of four full and four adjunct professors, including an additional research group headed by a permanent scientist. They cover a wide range of topics from basic theory, method development, applications in catalysis and life sciences, as well as machine learning. They have an excellent track record in all aspects, and they are the top group in Norway and one of the best at an international level. TheoChem provides facilities to develop codes for applications in the CTCC centre.

The Evaluation Committee considered the points raised by the administrative unit in their Terms-of-Reference document and have commented on many of the issues raised in that document. Where no comments are provided, this generally reflects a lack of relevant information in the selfassessment to allow the Evaluation Committee to reach a view.

## Recommendations

According to the research group assessments – and in contrast to the self-assessment – the administrative unit consists of several strong groups and some weaker groups. In the strategy discussion of the Department, it is mentioned that in these weaker sections, positions are going to be cut. However, these positions will be not shifted to the more successful sections but instead used to cut the overall budget of the administrative unit.

The Evaluation Committee believes that the outcome of the assessment for the section Organic Chemistry is particularly weak, which is a large section, and it is of great importance for the whole administrative unit. The main problem here is a recent and ongoing loss of highly reputed staff. Therefore, immediate action should be taken and – also suggested in the research group assessment – for example, external expert consultants could be involved to improve the overall situation. Organic synthesis could have very strong links to the medicinal arena at the interfaces of pharmacy/biology/medicine. In principle, the section could be a strong partner to the pharmaceutical

industry in the areas of drug discovery, drug synthesis, and drug development. This would be also an important complement to the orientation of some other sections of the administrative unit in the materials research area. In addition, this change could solve other problems of the section, and would also streamline and increase the internal collaboration, increase industrial collaborations, and finally could provide nice storylines for outreach activities.

Another issue identified by the Evaluation Committee (and deemed to be as important issue as the above proposed restructuring) is the fact that many retirements are coming up soon, which will also affect the strong sections of the administrative unit. It would be essential to develop a wise recruitment strategy with international committee members to fill crucial positions to sustain high level research in the future. This also includes potential offers to internationally known candidates should be competitive at an international level (salary, equipment, staff). Besides upcoming retirements and outside offers for staff, resignations of important PIs are further weakening the research performance of the administrative unit and will increase a downward spiral. This is particularly true for organic chemistry, radiochemistry, and highly needed medicinal chemistry. This is a major crisis with the potential that the new Life Science building cannot be used the way it should be. A national strategy for the future development of Chemistry in Norway is required to fill these gaps and in addition, a national funding strategy from RCN should be created to stop the brain drain in these particular areas. Otherwise, the Evaluation Committee believe that the momentum of the new Life Science building will fade away and could be a bad investment. Putting recruitment plans on hold or cutting down positions will be counterproductive and further weaken the administrative unit. It is also recommended that the administrative unit should not further diversify its structure (e.g. by hiring a new polymer chemist with high priority) but instead develop its existing structure with high level scientists. To establish new administrative units based on single scientists is much riskier than increasing the research power of broader administrative units with a smart recruitment strategy. The proposed goals of the Department are perhaps a bit too optimistic based on the overall level of resources and funding.

A summary of the recommendations provided by the Evaluation Committee is presented below:

- 1. High priority goals should include filling vacant positions, particularly in the areas of organic chemistry, radiochemistry, and medicinal chemistry (with the integration of pharmacy) to build up powerful research centre in the new Life Science building
- 2. High level recruitment of vacant position of leader of NMR centre (viewed as a great opportunity for new equipment in connection with Life Science building)
- 3. Improve possible commercialisation in several areas
- 4. Improve the amount of external funding secured
- 5. Improve the societal impact of the research outputs
- 6. Increase the number of female staff members
- 7. Discuss high teaching load of the administrative unit in comparison to other units

#### 1. Strategy, resources and organisation of research

The overall strategy of the administrative unit is described in detail in the self-assessment. However, the resource distribution will be changed in the future because of a proposed cut of appointments in the areas of organic and physical chemistry. Additionally, there will be no increase of appointments in the more successful areas e.g. inorganic materials chemistry, electrochemistry, and theoretical chemistry to compensate the cut of the other areas.

The up-coming recruitment strategy for the administrative unit is of great importance for future success. International participation in the recruitment committees should be organised. The level of

funding reflects the level of research quality, but the existing resources are not used properly from the weak sections of the administrative unit. The new organisation for UiO's priority areas and centres favouring thematic orientated science rather than disciplinary science provides a flexible tool to react on emerging and challenging research areas of societal and/or global technology needs.

## 1.1 Research Strategy

As pointed out in the self-assessment of the Department, high standards must be set in the quality of research and visibility of the research performed in the sections. This means a broad grant income from a variety of funding organisations and publication of the results in high level international scientific journals. The administrative unit follows the Research Council's shift from disciplinary science to more thematic science and this new strategy seems to sustain research income and proper use of resources.

The administrative unit is aware of the fact that the most active groups are also the most successful ones in bringing in grant money and producing high level scientific publications. Therefore, the administrative unit proposes a priority list of new advanced instruments to further support the scientific output in these groups. However, the administrative unit tries to balance this strategy to also support individuals with prospects for the future.

The overall research strategy of the administrative unit should make better use of the decision to get a new Life Science building. There should be a thoughtful strategy for the best integration of the groups active in this area and most likely could overcome the crisis of organic chemistry offering new perspectives for the future (e.g. a possible fusion with pharmacy to create a powerful new centre). As pointed out in the self-assessment "An outstanding Department of Chemistry...", a key for future success will be the recruitment of new faculty, because several key players will retire/leave the Department in the near future. There should be no doubt that these up-coming recruitments should be in challenging and "hot research topics", supporting the new infrastructure. Of equal importance is ensuring that the selection process is transparent and includes international participation to hire the best possible candidates.

## 1.2 Organisation of research

The administrative unit consists of a leadership of the Department of Chemistry (Head, Deputy Head, Head of Teaching, and Head of Office) and is divided into eight research sections, each headed by a Section Leader:

- Organic Chemistry (OrgChem)
- Inorganic Materials Chemistry (InorgChem)
- Catalysis (CatChem)
- Electrochemistry (ElChem)
- Chemical Life Science (Bioanalytical Chemistry, Structural Biology and Bioanalytical Chemistry (ChemBio)
- Environmental Chemistry (Nuclear Chemistry (NucChem), and Atmospheric Chemistry (AtmChem)
- Theoretical Chemistry (TheoChem)
- Chemical Didactics (ChemDidact)

Monthly meetings are scheduled between the section leaders to coordinate research and organisation. In addition, the head of teaching organises and conducts the teaching programs of the Department and coordinates it with the MN faculty. Furthermore, the administrative unit holds two educational programs (both offering B.Sc. and M.Sc.) each having a program leader. In theory, the

organisation of the administrative unit sounds reasonable, but from the actual situation of the Department, it gives the impression the organisation suffers from a lack of clear decisions, and the overall management is rather weak.

## 1.3 Research funding

The funding situation of the administrative unit depends very much on the source of funding. In general, funding from national sources (RCN) is on a good level and quite distributed between the research sections. However, external funding is quite limited and large differences are observed between research sections. External funding offers the possibility to hire PhDs and post-docs from outside to ensure more innovations and future technologies.

In summary, from 180 FTEs at the administrative unit 127,9 FTEs were successful in securing general national funding. The situation for external funding is very different and only a few grants have been granted to some sections of the administrative unit. The majority of funding is provided by RCN (64 711 725 NOK). International grants, e.g. EU, international industry (9 644 502 NOK) are much lower and are in the range of less than 15% of the total budget.

#### 1.4 Use of infrastructures

The administrative unit relies on the use of high-level instrumentation to carry out its research. Most of these instruments have been financed by RCN and UiO over the last decades.

On a national level this includes X-ray, NMR, computing and data storage, transmission electron microscopy, battery characterisation, proteomics, and microfabrication. Again, the new Life Science building will bring up opportunities to get top level new instrumentation to increase their national significance.

A minority of high-level instruments are also used on an international basis provided by special contracts (e.g. Swiss-Norwegian beamline, see below). UiO manages research data according to international standards, such as the FAIR principles.

## 1.5 National and international collaboration

The administrative unit states that national and international collaboration is very important in terms of high-level scientific publications, but it is not formalised in a administrative unit strategy, and it is mostly based on individual connections. They have access to international synchrotron facilities in connection with new material research and structural biology. These groups are regular users at the Swiss-Norwegian beamline (SNBL) at ESRF (Grenoble), where Norway is a co-owner, and the administrative unit is represented at the board.

Political means for collaboration and interdisciplinary work are institutionalised within the university and various EU programs.

As a result of the international activities, 71% of the administrative unit's publications between 2019 and 2021 were co-authored with international collaborators, which is in line with the average for Norwegian universities in the natural sciences.

## 1.6 Research staff

The distribution of the research staff follows a typical pattern: around 50% of the PhD students are female, whereas only 25% of the permanent scientific staff (Prof. and Assoc. Prof.) are female. This is being addressed by the administrative unit through the FRONT project on equal opportunity, hosted by the faculty. The management of the administrative unit and the leaders of the sections are enrolled in a running program of four half-day seminars on the issue. The administrative unit actively uses its international PhD fellowships (KD-stipendiary) in a strategic way to increase the number of international high-level students. In addition, RCN has established the Young Research Talent program to further support young researchers. The section for researcher support at the faculty provides excellent administrative services for ERC starting grants and mentoring research proposal writing.

The high proportion of technical staff to scientific staff can be explained by the complexity of chemistry in teaching lab courses and setting up complex experiments.

The productivity of women and men within the administrative unit, measured as the average number of author shares by FTE, differs slightly: in the period 2019-21, female members of the administrative unit have an average author share of 1.19, whereas their male colleagues have an average of 1.31. Compared to some other administrative units in the evaluation, the difference is rather small, but there is nevertheless room for improvement.

## 2. Research production, quality and integrity

The administrative unit tries to set the highest academic standards publishing in highly visible scientific journals and securing competitive research funding – at least on a national level. The overall research production of the administrative unit is high but not all units provide equally at the same quality level. The administrative unit will be confronted with major problems in the near future because the economic situation has forced the Department to cut seven positions within the next five years. In addition, several key players and research leaders will retire at the same time. The most productive research groups InorgChem, CatChem and ElChem will be not affected by the cuts. Finally, the TheoChem group and the AtmChem group will get an extra associate professor position.

UiO researchers are obliged to familiarise themselves with and perform their research in accordance with the recognized scientific and ethical standards applicable in the field. UiO has established a Standard for Research Integrity.

## 2.1 Research quality and integrity

#### Atmospheric Chemistry research group overall assessment

Although the size of the Atmospheric Chemistry group has been smoothly growing since the appointment of a professor of atmospheric chemistry in 2014, it is still really very small, especially taking into consideration the scientific nature of Atmospheric Chemistry. The small size also poses challenges for the future viability of the group. The research of the group covers a range of different topics all the way from global atmospheric studies to, theoretical studies and from instrument developments to applied studies. The research is mainly of quite high quality, but a larger group size would give the talented group members better possibilities to catalyse their thoughts, ideas, and discoveries. it would also strengthen the collective leadership with less dependence on one individual and minimise overloading the leader of the group. Critical mass would allow also better training and

support of early-career researchers (PhD students and postdocs) and new courses on atmospheric chemistry would attract talented students to carry out PhD studies.

#### Catalysis research group overall assessment

Based on international comparison, this group is strong, but possibly not the strongest worldwide. Very high peaks of excellent quality are visible, but a more comprehensive strategy of the group is needed to maximise the impact.

The strengths of the group include PIs with excellent track records and complementary expertise and very good publication records. In addition, this research group is active in important and current topics and in many international consortia, often in a leading role. They also have very good knowledge transfer strategies for some areas of their research. The weaknesses of the group are that homogenous catalysis activities appear to be weaker than the heterogeneous catalysis work, especially given that the senior professor is close to retirement. Overall, the weakest point of the group is the section on societal impact, which is in the average, without going above expectations.

#### Chemical Life Sciences research group overall assessment

The Chemical Life Sciences group of University of Oslo has made significant contributions to the field. This group is an excellent example for best practices with respect to research and organisation. Its vision with the new building will further support this. The group has a strong focus on biomolecules, bioanalytics and biomaterials, and demonstrates this. The Evaluation Committee noted that the output of the individual groups is great, however more collaboration between the groups is suggested. Only a few projects or publications have been listed from more than one group member. The SWOT analysis is a bit short, and mainly claims that a weakness is too much teaching. The Chemical Life Sciences group is very well positioned for the future and has developed an excellent scientific quality in most of its activities. Slightly more structured and focused approaches to target its scientific goals would be beneficial. Furthermore, the societal impact of its research is a weaker issue. Here the Chemical Life Sciences group should expand its industrial collaboration.

#### Electrochemistry research group overall assessment

This is a strong group covering a wide scope of research activities in the areas of solid-state electrochemistry, electrocatalysis, and photoelectrochemistry. The research performed by this group is of excellent quality and is internationally recognised, as reflected by the publications in high impact factor journals.

The group is a pioneer internationally with its discovery of proton conduction in ceramic materials at elevated temperatures.

The group is clearly reaching its objectives of high-quality research, high visibility in Norway and internationally. The success in acquiring third-party funds is outstanding and does not surprise given the high importance of the topic. This allows the research group to be very strong regarding the number of young scientists (PhDs) working on different aspects of the topic. Applications of the research to advanced functional materials and nanotechnology for sustainable energy have a significant societal impact.

#### Inorganic Materials Chemistry (NAFUMA) research group overall assessment

The NAFUMA team at UiO is a rather small administrative unit with three professors and two assistant professors. As said, there is no strict organisation regarding the research topic, however the team is organised including regular meetings and co-supervising of students.

In the self-assessment the research group gave rather ambitious goals, such as becoming a leading group in Norway and at UiO within the fields of solid-state chemistry, inorganic materials chemistry, and nano chemistry, with relevance for energy, environment, and sustainability. In addition, they want to strengthen their existing expertise and experience in in-operando studies by use of synchrotron and neutron large scale facilities. The external funding secured is good and the scientific output is very good. The group is also responsible for the RECX lab (XRD national infrastructure), thus providing a service structure for partners from academia and industry. To complete the picture, NAFUMA researchers are strongly involved in teaching and drivers of the MENT/ MENA (Materials, Energy and Nanomaterials) study program, as well as other outreach activities including industrial partnerships, patents, starting of a spin-off company, and science to public activities. However, the ambitions seem to be unbalanced to the resources presently available.

Overall, the group is well-positioned in the UiO strategy on materials, nanoscience, energy, and sustainability, however the team sees itself in a critical situation regarding young talents and junior staff, as well as funding and maintenance of the high-end research infrastructure. The up-coming retirement of one of the key researchers probably also plays a role in the critical perception on how to proceed.

#### Organic Chemistry research group overall assessment

Overall, the OrgChem research group is loosely organised around three subgroups working in NMR spectroscopy, organic synthesis, and radiopharmaceutical chemistry. It displays strengths in NMR spectroscopy (as an active collaboration partner in high-quality consortia), including the provision of services to external partners, particularly from industry. The group has also made commendable efforts in public outreach activities. While OrgChem's work in organic synthesis has had some highlights, https://web.archive.org/web/20150316083902/https://royalsociety.org/awards/davy-medal/ the impact and productivity of this research field are on a downward trend. The Evaluation Committee notes weaknesses in the research outputs of the radiopharmaceutical subgroup, and a downward trend in the research productivity of the other subgroups. The Evaluation Committee notes with particular concern the disintegrating personnel situation, which mandates immediate and serious action and a coherent recruitment and development strategy. The Evaluation Committee thus disagrees with the group's repeated assertion that it is the leading synthetic organic chemistry group in Norway. While the group has made important contributions to the institution and to society, its role in advancing the state of the art in organic chemistry in a modern sense is dwindling.

#### Theoretical Chemistry research group overall assessment

The main impression of the Evaluation Committee related to the Theoretical Chemistry RG at UiO is that this is a top group in Norway and internationally. The strengths include excellent research groups in areas covering a wide range from basic theory, method development, applications in catalysis and molecular life sciences, as well as machine learning. Importantly, these groups also collaborate within the RG, in the UiO chemistry department and internationally. There is a well-structured communication within the RG in terms of science and science management. The important tasks for the future development of the group are to further increase scientific discussions between the groups, specifically also including the groups involved in electronic structure calculations, applied computational chemistry and machine learning; to maintain the high standards, i.e. to keep a top position nationally and internationally in terms of creativity and productivity in the field of theoretical chemistry. An important task in this respect is to appoint top scientists both in fundamental and applied computational chemistry. The main weakness of the group is in terms of outreach and communication with society.

## 2.2 Open Science

The UiO has an open science policy stating that all members of staff should do their best to ensure that scientific articles deposited into the institutional repository can be made openly available as soon as possible.

According to the available bibliometric data, 18% of publications in 2021 were published in Gold OA, and a further 65% in Green OA; 17% of publications are not available in Open Access. This puts the administrative unit slightly above the average for Norwegian universities in the natural sciences (Gold OA: 32%, Green OA, 48%, non-OA: 20%).

## 3. Diversity and equality

In the self-assessment of the administrative unit, it was expressed that KI strictly follows the rules of UiO promoting equality and diversity. Students and employees shall be included in a safe study and work environment that brings out the best in everyone. It appears as though these regulations fulfil best international practices. Finally, all recruitment plans are based onto these regulations with high priority of gender issues.

At UiO, students and employees are encouraged to report any censurable condition or behaviour they experience.

## 4. Relevance to institutional and sectorial purposes

The commercialisation efforts of the administrative unit are quite broad and cover both early-stage research by the establishment of a so-called "Growth House", where early-stage research ideas will be focused into a possible business direction, and secondly already more developed business ideas to be transformed into a possible business by a "University Tech Transfer Office" including managing IP issues. This covers the whole education program of the administrative unit from bachelor's to master's and finally PhD candidates. Finally, a science park is available to support start-up companies.

In summary, the idea of technology transfer of basic research into a business model are handled quite straight forward at the administrative unit but however, the success rate should be improved.

## 5. Relevance to society

The relevance of the research of the administrative unit to society is very impressively demonstrated by the impact cases presented by the self-assessment of the administrative unit. All three cases are important contributions to Norwegian society and should have a long-term effect. In particular, the  $CO_2$  capture project deals with a global societal challenge and tackles an important problem of the global climate change and could be part a solution against global warming.

The second case deals with catalysis and also covers a very challenging issue for the future direction of chemical industry and future production of new materials.

The third case is theoretical in nature but has the potential to shift into the direction of applied sciences; the theoretical design of new catalysts could be used for future applications in chemical industry.

Comments to impact case 1: Environmental impact of amine-based CO<sub>2</sub> capture

The AtmChem group at the administrative unit has a long history in the amine-based  $CO_2$  capture. This turns out to be very important following the climate change discussions on a high political level.

The group has developed analytical methods on amine emissions and degradation of amines to carcinogenic nitrosamines and was therefore able to set-up a large-scale project on  $CO_2$  capture based on amines showing that only very minor emissions and degradations took place. Unfortunately, the project was stopped for economic reasons, but luckily the group did not give up and continued their research efforts in the area.

In 2020 Norway decided to implement the world's first full-scale CO<sub>2</sub> capture, transport and storage project which includes two full-scale amine-based CO<sub>2</sub> capture plants.

This impressively demonstrates that basic research can result in a very important industrial process. It also shows that the standing of the individual researcher is most important for the success of a project that was almost stopped some years ago.

#### Comments to impact case 2: UiO 66 metal organic frameworks

This important research has been performed in the catalysis section of the administrative unit over the last few years. It combines inorganic research on porous inorganic materials (zeolites) and its further development into metal organic frameworks (MOFs). In a very successful way the expertise in inorganic synthesis and structure, organometallic and organic synthesis, and heterogenous catalysis was used to generate the impact.

The successful development is demonstrated in a number of scientific papers and patents. The findings resulted in unprecedented chemical and thermal stability, as well as tuneable porosity. The X-ray structure could be also solved via a European collaboration and the organic synthesis expertise in the section resulted in modified MOFs by organic synthesis to develop custom made linkers to create tailored materials.

Finally, important applications emerged, including hydrogen storage and high temperature heterogenous gas phase catalysis. Ni-functionalised UiO MOFs were used as catalysts for ethene dimerisation and Pt-functionalized materials for CO<sub>2</sub> hydrogenation.

In summary, this is a great showcase with tremendous impact in various areas of chemistry.

#### Comments to impact case 3: Dalton quantum chemistry program system

Dalton is a powerful general-purpose open-source program system for the study of molecular electronic structure at various levels of theory. Scandinavia has a long tradition of collaborating in quantum chemistry and in provide powerful tools for *ab initio* molecular electronic-structure calculations. It is being used successfully by thousands of chemists around the world, as Dalton was made open source in 2017. The members of the theory section at UiO have contributed to Dalton in a number of ways. Regarding the theoretical developments underlying Dalton the UiO group has contributed to second-quantisation formalism for perturbations, methods for calculating time-dependent properties, molecular magnetic properties, the Lagrangian method for nonvariational wave functions, derivative integral evaluation, geometry optimisation, and direct *ab initio* dynamics. Besides that, the group has also contributed to several parts of the Dalton code and finally the feature of an *ab initio* calculation of an NMR spectrum for the first time.

## List of administrative unit's research groups

Institution	Administrative Unit	Research Groups
University of Oslo - Faculty of Mathematics and Natural Sciences	Department of Chemistry	Chemical Life Sciences
		Electronics Research Section
		Catalysis Section
		Theoretical Chemistry
		Inorganic materials chemistry (NAFUMA)
		Organic Chemistry
		Atmospheric Chemistry

## Methods and limitations

#### Methods

The evaluation is based on documentary evidence and online interviews with the representatives of administrative unit.

The documentary inputs to the evaluation were:

- Evaluation Protocol (see appendix 3 Evaluation Protocol) that guided the process
- Terms of Reference
- Administrative unit's self-assessment report
- Administrative unit's impact cases
- Administrative unit's research groups evaluation reports
- Bibliometric data
- Personnel and funding data
- Data from Norwegian student and teacher surveys

After the documentary review, the Evaluation Committee held a meeting and discussed an initial assessment against the assessment criteria and defined questions for the interview with the administrative unit. The Evaluation Committee shared the interview questions with the administrative unit two weeks before the interview.

Following the documentary review, the Evaluation Committee interviewed the administrative unit in an hour-long virtual meeting to fact-check the Evaluation Committee's understanding and refine perceptions. The administrative unit presented answers to the Evaluation Committee's questions and addressed other follow-up questions.

After the online interview, the Evaluation Committee attended the final meeting to review the initial assessment in light of the interview and make any final adjustments.

A one-page summary of the administrative unit was developed based on the information from the self-assessment, the research group assessment, and the interview. The administrative unit had the opportunity to fact-check this summary. The administrative unit approved the summary with minimal adjustments.

#### Limitations

(1) The Evaluation Committee judged the information received through documentary inputs and the interview with the administrative unit generally sufficient to complete the evaluation.

## Appendices (link to website)

- 1. Description of the evaluation of EVALNAT
- 2. Invitation to the evaluation including address list
- 3. Evaluation protocol
- 4. Self-assessment administrative units
- 5. Grading scale for research groups

Website: https://www.forskningsradet.no/tall-analyse/evalueringer/fag-tema/naturvitenskap

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