Universitetskanslersämbetets utbildningsutvärderingar

Self-evaluation

Lärosäte	Uppsala universitet
Forskarutbildningsämne	Kemi med inriktningarna Fysikalisk kemi och Kemisk fysik
Licentiatexamen	Ja
Doktorsexamen	Ja

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1. Background description

This self-evaluation was made jointly by all supervisors in the two subjects *Chemistry with specialization in Physical Chemistry* and *Chemistry with specialization in Chemical Physics* (henceforth referred to as "*Physical Chemistry*" and "*Chemical Physics*", or the "subject(s)") Input from the doctoral students was provided mainly during late 2019 and spring 2020, following the original time plan from UKÄ. We chose to write the document in English to be able to include all supervisors in the process. Thus, we could use this opportunity for a broad discussion and reflection on our PhD education in the supervisor group. To ensure input from all presently active students, while minimizing the time requested from them, we conducted a survey in December 2019 (all PhD students responded). This was done when the self-evaluations were due in the spring of 2020. The results are referred to in the text. All supervisors worked in small groups to create content and write text for the different sections, followed by cross-reading and feedback on the parts from the other groups. The Professor responsible for Third cycle studies with specialization *Physical Chemistry* and *Chemical Physics* (FUAP) collected a complete draft, and updated this in September 2020. All supervisors and two volunteer doctoral students read and commented on this version, and adjustments were made. The UU central Unit for Quality and Evaluation read the resulting version, and after their feedback, we completed the self-evaluation during November 2020.

List of Surveys and Evaluations we used and refer to:

- Our own PhD student survey (Dec 2019)
- Department work environment survey 2020 (summary for the Physical Chemistry program)
- Department alumni survey 2018
- UU Quality and Evaluation unit survey with report for our Faculty 2017.
- UU-wide evaluations "Quality and Renewal" ("KoF") 2011 and 2017

Definition of the subject

"Physical chemistry is everything that is interesting and exciting!" is a quote often attributed to G. N. Lewis. While there are many different definitions of the discipline, it is characterized by the use of physical theory, models and methods in the study of chemistry. Compared to most other chemistry disciplines, it is thus defined by its approach rather than by the nature and identity of the systems studied. Chemical physics often overlap with physical chemistry, but its origin as a branch of physics emphasizes its distinction by the systems and phenomena studied, while the physics approach is given from the start. Our research in physical chemistry/chemical physics is summarized in the next sub-section. It often inter-disciplinary, with strong elements of organic-, inorganic- and biochemistry, as well as physics, mathematics, pharmaceutical and material sciences. We collaborate extensively with other disciplines at neighbouring research programs within our Department and the Departments of Physics and Astronomy, Mathematics, Technology, Pharmacy and Chemistry - BMC, as well as internationally.

The *Physical Chemistry Research Program*

Research at the Faculty of Science and Engineering ("TekNat") at UU is organized in 64 *Research Programs*, which are organizational units within TekNat. There are nine Research Programs in the Section of Chemistry. Each supervisor and doctoral student belong to a Research Program, which is the environment where doctoral students work and study. The Physical Chemistry program has 19 PhD students and 12 supervisors. In our case, we have extensive collaboration and daily interactions with PhD students and supervisors from other Research Programs and PhD Subjects. Most of the faculty financing for research and third-cycle studies (ca. 70%) is directed to the programs. Each program has a responsible professor, with the responsibility to create and maintain a research environment of high quality with competence for education and supervision at all levels.

The third-cycle studies are organized in *Subjects* (*e.g. Chemistry*) often with *specializations* (*e.g. Physical Chemistry* or *Chemical Physics*), where each specialization has a responsible professor ("FUAP"). In our case, the FUAP for both subjects of this self-evaluation (Hammarström) is also responsible for the program.

The Physical Chemistry Program conducts both fundamental and goal oriented research related to chemical dynamics, surface & colloid chemistry and solar energy conversion. Our research is focused on:

Solar cell materials and devices. We design and develop new dye-sensitized, quantum dot, plasmonic and perovskite solar cell systems such that they are more efficient, low-cost and environmentally friendly. We do fundamental photophysical and electron transfer studies using advanced electrical, optical, and X-ray measurements to delineate mechanisms of energy conversion. Devices are fully characterized and tested for stability under simulated terrestrial light conditions.

Artificial photosynthesis. We develop new photochemical systems that use light to drive charge separation and catalytic reactions (e.g. H^+ and CO_2 reduction) that produce "solar fuels." We design and study solid-state, molecular, and protein systems that undergo (multi)electron transfer (ET) and/or (multi)proton-coupled electron transfer (PCET) in the context of catalysis, where mechanisms are resolved with optical and IR transient spectroscopy and electrochemistry. Effective water splitting and CO_2 reduction devices have been made by merging molecular and solid-state catalysts with a variety of photosystems, such as dye-sensitized semiconductors, quantum dots, polymeric and carbon dots and plasmonic nanoparticles.

Chemical dynamics. We use transient UV/VIS/mid-IR femtosecond laser spectroscopy as well as X-ray absorption and scattering spectroscopy to probe ultrafast structural dynamics and electronic changes in small molecule, protein, dye sensitized semiconductors and solid-state systems. Atomic telemetry, a new method using resonant X-ray emission spectroscopy and molecular dynamics simulations has been developed. We use computational methods to study diffusion in complex and crowded systems.

Surface, Colloidal and Macromolecular Chemistry. Research in surface and colloid chemistry includes a group with focus on fundamental and applied studies of self-associating lipid and surfactant systems. The group is localized on BMC and work mainly with questions of biological, pharmaceutic and medical relevance. At Ångström, a group develops novel and more efficient methods for computational studies of complex colloidal and polymeric materials to explain and predict e.g. surface properties of polymers and transport of nanoparticles and macromolecules in polymer gels.

Our focus on renewable energy research is well aligned with the University's commitment to *energy and sustainable development*, and several of the UN sustainable development goals. Further, the Physical Chemistry research program enjoys high international visibility, a breadth of interdisciplinary expertise, and attracts a large number of guest students at all educational levels. We constitute a strongly international environment, with many projects of high international visibility.

Third-cycle (PhD) education.

Research and PhD education in the physical chemistry program has an annual turnover of ca. 41 MSEK, and is financed by ~37% from faculty funds and ~63% from external funds (from Budget 2020). Uppsala University has conducted research education towards a doctoral (PhD) degree in *Physical Chemistry* for a long time. The Svedberg was the appointed as the first Physical Chemistry Professor in Sweden in 1912 (Nobel Prize in 1926), and he supervised 18 students to PhD degree 1913-1949. One of them was Arne Tiselius, who was awarded his PhD in 1930 (Nobel Prize in 1948). Since 1998, 54 students have been awarded a PhD in Physical Chemistry (or "Chemistry with specialization Physical Chemistry" after 2010).

The PhD subject area (specialization) *Chemical Physics* was introduced in 2006, at the same time as a Research Program in Chemical Physics was created. This was connected to changes in department structure within the Chemistry Section at UU. Since 2007, 16 students have been awarded a PhD in Chemistry with specialization in Chemical Physics. In 2012, after further reorganization of the Chemistry Section into two departments, the Research Programs *Physical* Chemistry and *Chemical Physics* joined the same department and decided to merge into one Research Program, under the name *Physical Chemistry*. The PhD subject area of *Chemical Physics* remains, to suit students with a previous training mainly in Physics/ Engineering Physics. In practice, the two subjects, the third-cycle training and the doctoral students groups, as well as the supervisors, are completely integrated. Therefore, this self-evaluation describes the joint environment and third-cycle studies of the two subjects. The PhD students also work in close collaboration with researchers in other programs and PhD students in other subject areas (Section 2.2). In 2010, the TekNat faculty changed the titles of our subject areas to "Chemistry with specialization in…" This was a pure formality and of no practical consequence.

There are three levels of study plans for third-cycle studies at UU: the general study plan, the subject-specific study plan and the individual study plan (ISP). After the latest revision of subject-specific study plans in 2016, there are no differences in the contents for the two specializations *Physical Chemistry* and *Chemical Physics*. Today, the new students have the possibility to choose between the two subject areas depending on their educational background and identity. We have discussed within the program if we should simply merge the two specializations. We recently (Jan 2020) decided to instead keep both specializations and make their plans distinct again to reflect the different student backgrounds and identities. We will then also include descriptions of the respective research areas of Physical chemistry and Chemical physics. This is a point for development and improvement during 2021.

Organization of the PhD education.

The ultimate responsibility for the third-cycle program at the University rests with the University Board and Vice Chancellor, who have delegated certain responsibilities to the various Disciplinary Domains and Faculty Boards. Although the overall responsibility (including monitoring responsibility) rests with the Disciplinary Domains and Faculty Boards, operational responsibility for any given third-cycle student rests with the department at which the student is registered. The Disciplinary Domain, Faculty and Department Boards, along with the supervisors, bear the responsibility for third-cycle programmes being run in a manner characterised by high quality, efficiency and respect for the rights and responsibilities of all concerned. The Faculty Board of Science and Technology thus bears the overall responsibility for the Faculty's third-cycle programmes. The Faculty determines which subject areas are to be the focus of such programmes as well as the general content and design of the study plans. The Faculty's Graduate Educational Board (*Forskarutbildningsnämnden, FUN,* in Swedish) handles ongoing issues and makes decisions (under authorisation by the Faculty Board) concerning the establishment of subject area/specialisation study plans, etc.

The TekNat Faculty webpage is a great resource of well-structured and useful information that collects all documents, rules and regulations regarding third-cycle studies that are needed, from admission to examination: https://www.teknat.uu.se/education/postgraduate/

Third-cycle education is carried out at the departments. For each specialization, the Faculty Board approves a study plan and a professor responsible for third-cycle education (*forskarutbildningsansvarig professor, FUAP*) with overall responsibility for development and quality-control of the subject / specialisation. Each department has a Director of studies for third-cycle programmes whose duties are specified by the Faculty Board and who is authorised by the Head of Department to provide active support, relating to a range of issues, to the department's third-cycle students as well as to supervisors and professors responsible for third-cycle education, regardless of subject area/specialisation. One department administrator is dedicated to third-cycle studies administration, to aid the Director of studies. The third-cycle studies have several components contributing to supervision, planning and evaluation:

Supervision. Every PhD student has one main supervisor (who must have undergone the required pedagogic/supervisory training) and at least one co-supervisor. The main supervisor is responsible for the planning and evaluation of the student's progression and fulfilment of goals, including the thesis, together with the student. The Individual Study Plan (ISP) is a useful support in that work.

Supervisory group. This is the group of all twelve supervisors in the Program (Section 2.1). We meet once per year to go through PhD student progress and the updated ISPs. We meet during informal lunch meetings about once per month, where PhD studies and supervision is a frequent topic of discussion. This group is vital for development and improvement of individual supervisors and of the third-cycle education in general.

Study plans. The PhD study plans are at three levels: A general plan for all PhD studies at TekNat, a subject specific plan (Physical Chemistry or Chemical Physics), and the Individual Study Plan (ISP) for each student. The latter is revised and updated at least once every year, before October 15. All students and supervisors must go through, discuss and evaluate progress, and make plans for the future. To ensure that the studies are progressing towards the Examination Goals of "Högskoleförordningen" (HF), the goals are written into the ISP form, and the ISP must state what progress has been made towards each goal, and give concrete examples of activities to make that progress. Similarly, the planned progress for the coming year must be briefly described. All revised ISPs are signed by the students, all supervisors and FUAP. Important formal changes (e.g. change of supervisor or dissertation date) require a signature from the Head of Department. All ISPs are stored by the department administration and reported to the TekNat faculty.

We are following up each ISP yearly, in the Supervisory group of all supervisors in the program. We discuss general challenges as well as individual ones, and decide on actions. In cases problems arise that cannot be solved by the supervisors and student themselves, the FUAP and the Supervisory group can function as external support. In individual cases, this could mean an increased frequency of supervisory meetings, sometimes including a senior who is not involved in the scientific project, to give "third party" input. This has worked well for students that have problems in structuring their work and/or feel low self-esteem. Involvement of an impartial advisor can help getting a sense of seriousness about structured work, or help lifting confidence when confirmed by an independent senior. If more serious problems or conflicts arise, the student and supervisors can turn to the Study Director for third-cycle studies or the Head of Department. If this does not work, help can also be provided by TekNat's committee for third cycle studies (Forskarutbildningsnämnden, FUN).

Recruitment of PhD students. The need and possibility to announce a PhD position is identified by the potential supervisors, typically in connection to funding of a research proposal, the employment of a new Professor/Researcher, or other needs. Discussions with the Program Professor and Head of Department follows. Our routines for recruitment of PhD students follow the rules of UU and TekNat. Since 2019, we follow new Department routines. All positions are advertised openly, through the UU website and other channels, such as professional societies and informal research contacts. All top candidates are invited to structured interviews, preferably on site, by a group including at least the main supervisor, one professor who is not involved in the intended research project, and one person from HR; gender representation is considered in selecting the group. The interview may include a scientific task (e.g. write an abstract to a manuscript or summarise a few papers). Many candidates have instead done an exchange project (Erasmus) or Master project with us, and this is obviously an important possibility to assess the candidate's practical and scientific skills. The group discusses and agrees jointly on the best candidate, but the intended supervisor of course has to agree with the group decision.

The fraction of international PhD students (with a foreign undergraduate degree) at TekNat increased from ca. 50% in 2008 to ca. 80% in 2018. Chemistry and our specialization has followed the same development. The number of internal (UU) candidates have dropped substantially during the same time, even if the number of 1st and 2nd cycle students has not decreased. It is a challenge to reach good PhD candidates with advertisements for open positions, as undergraduate students are not members of professional societies and networks to the same extent as e.g. postdoc candidates. Often the interesting candidates are reached, or reach out to us, via our personal research networks. Our Master program in Chemistry, with many international students, has gradually become an important recruitment base.

Follow-up and evaluations. We have a structured range of activities for following up PhD student progress, in addition to the IPS revisions, and for the evaluation of research and third-cycle studies; this is described in the sections below.

2. Preconditions

2.1 Academic staff

Assessment criteria:

The number of supervisors and teachers and their combined expertise (scholarly/artistic/professional and pedagogical) are sufficient and proportional to the volume, content and implementation of the programme in the short term and long term.

The number of supervisors in the *Physical Chemistry* research program is twelve, where eight are male and four are female, see Table 2. Among those, four are Full Professor, four are Senior Lecturer ("Högskolelektor"), two are Assistant Professor ("Forskarassistent") and two are Researchers. Of the 12 supervisors, four have PhD´s from UU, one from GU and six from other countries (China, Germany, The Netherlands, Spain, UK and the US). Nine of these have the title of Docent. We have also a number of professors and researchers as supervisors from other departments and programs, see table 3. As a complement, many other researchers and postdocs function as support, with close experience and knowledge of the labs.

The supervisors have time to dedicate themselves to research and supervision. Eleven out of twelve of the supervisors in the *Physical Chemistry* research program have at least 60% of full time for research and supervision.

The number of supervised PhD students in the subjects *Physical Chemistry* and *Chemical Physics* are 19 (Sept. 2020), where ten are female and nine are male, giving a ratio of students/supervisors = 1.6. No one is main supervisor for more than four students. Thus, we have sufficient capacity to supervise more students, if funding were available. We also have the numeral and the breadth to handle a potential need for a change of supervisor.

Scientific competence. The scientific competence of the supervisors and teachers of the Program is high, with both breadth and depth in Physical Chemistry and Chemical Physics. The Program has a strong publication record; from 2010-2017 (data from the UU evaluation KoF 2017) we published ca. 570 articles, which equate to 330 points in the Norwegian model (the highest within the Chemistry Section). Many publications appear in high impact journals like *Science*, *Nature Chemistry*, *Nature Photonics*, *Accounts of Chemical Research*, *Angewandte Chemie*, *Journal of the American Chemical Society*, *Chemical Science* and *Energy and Environmental Science*.

We attract significant funding (63% of our research budget) from external grants: from Jan. 2012 to May 2020, we have received 99 grants comprising in total over 207 MSEK funding. Only since Jan 2019, we have received 30 grants of in total 65 MSEK. The most important sources are *VR*, the *Energy Agency* and the *K&A Wallenberg Foundation*, each contributing 40-50 MSEK since 2012.

We currently have eight project grants from VR (plus two postdoc grants), two project grants from the K&A Wallenberg Foundation and one Wallenberg Fellow grant, in addition to several grants from H2020 (FET-Open, MSCA…) the Energy Agency, SSF and VINNOVA.

We are all active conference participants within our respective fields. Since 2012 we have given nearly 100 invited talks and 20 keynote/plenary talks. We have organized prestigious international conferences (e.g. Gordon RCs), and founded the biannual International Conference on Solar Fuels with (500 participants in 2015).

Important factors are also the supervisors' and teachers' international networks. A higher quality leads to an increased selection of applicants for PhD positions and larger possibility to find a suitable candidate. Many supervisors have projects financed by VINNOVA, EU or SSF where companies are involved, or have direct financing from companies. Three supervisors have started their own companies. We routinely serve as committee members for PhD defenses and have been PhD opponent at European Universities at least 11 times since 2012. We frequently serve on international and national grant evaluation committees, such as in ERC, EU, Department of Energy (USA), NCN-Poland and VR. We (Hammarström) represented the Swedish Partner (UU) in the FET-Flagship initiative "SUNRISE" focused on solar energy for sustainable fuels and chemicals (www.sunriseaction.eu) now converted to SUNERGY Large Scale Initiative towards Horizon Europe. At ELI (Czech Republic) Sá coordinates the development of an X-ray spectroscopy end station. He also maintains extensive collaborations with ICFO Spain, SwissFEL, XFEL Germany, IFJ-PAN Poland, and TU Berlin. Sá sits on the panel to promote ELI-ALPS in Sweden. Several of the supervisors have international collaboration grants and agreements.

Pedagogic competence. All Associate Professors ("Lektorer") by recruitment or promotion must have taken ten weeks of university-level pedagogic courses, at latest within two years of employment. All staff and PhD students who teach on our first- and second-cycle courses must take at least the 7.5 cr course "Basic training for university teachers". The interest in chemistry education is strong at our Department, and in our Research program, and most students and supervisors are involved in both formal and *ad hoc* discussions on teaching and education. Pedagogic competence is visible and enhanced by structured teaching and interest for questions concerning didactics. A particular mention should be made to the pedagogical and didactic development work performed by our Associate Professor Maja Elmgren, and her book (*Academic Teaching* By: Maja Elmgren and Ann-Sofie Henriksson) that is used in basic pedagogic training courses at Uppsala University. We have received several internal UU grants for pedagogic and educational development projects, some of which have involved Master or PhD students. Two of our Associate Professors have been awarded the title "Excellent Teacher". All teaching at PhD courses, Master and Bachelor levels are conducted by teachers who also are active researchers. That is reflected in the choice of lectures examples, seminar questions, projects in courses and elaborative tasks. This will prepare both undergraduate and PhD students for the future career in both industry and academia.

We are strongly involved in teaching on a first-cycle level, as well as on Master level. Most PhD students teach on first-cycle level, mainly as lab teachers but in some cases also in classes (Problem solving). On the Master level, we are involved in particular in the Master program directions *Physical Chemistry*, *Theoretical & Computational Chemistry*, and *Chemistry for Renewable Energy*. The latter is one of the most popular directions in the Chemistry program, an all three directions are strongly coupled to our research and PhD education. Many advanced Master courses are taken by PhD students as part of their third-cycle studies (e.g. Laser Spectroscopy; Advanced Electrochemistry), and we offer specialized PhD courses such as *Fluorescence spectroscopy*, *Polymer physics* and *Electron transfer*.

Supervisory competence and development. All PhD supervisors have the required pedagogical education, including the courses "*Pedagogy for supervisors*" (5 cr), "*Supervising PhD students*" (5 cr) and "*Basic training for university teachers*" (7.5 cr), in total 17.5 credits. The older supervisors (>50 years old) have taken previous versions of pedagogic and supervisor courses.

Development of supervisor competence is done through supervisor meetings and workshops organized by the Study Director of third-cycle studies, once per semester. Topics that have been discussed during 2018-2020 include: Admission procedures and interviews, ISPs and how to use them, Procedures for follow-up of individual progress, Career planning, Extent of long-term sick leave, Gender equality on supervisor level, and the UKÄ evaluation. In addition, meetings for all FUAPs are organized by both the TekNat

Faculty (yearly) and our Department (once/semester). In addition to topics like those above, formal matters, rules etc. are discussed.

In the physical chemistry program, supervisors discuss supervision extensively in the *Supervisory Board* (Section 1), during two half-days per year when we jointly follow up the progress of each student. We also have lunch meetings about once per month, and often discuss aspects of doctoral training. This allows us to discuss ideas and current problems, and allows us to develop as supervisors through peer-to-peer exchange and discussions.

In our own survey among the PhD students (Dec 2019) the students agreed to a very high extent that their supervisors are scientifically very competent and have sufficient pedagogic competence to work well as supervisors. They thought that they get sufficient supervision time, and that it is easy to get more time if they need.

Continuity. Since 2012, two of the full Professors, one Senior Lecturer and two Assistant Professors have been recruited. During the same time, the number of Researchers (”Forskare”) have decreased and three full Professors retired or moved. Some of the previous Researchers have moved to other jobs, while others have successfully competed for openly announced Senior Lectureships. Four of the recruitments since 2012 have been on the assistant professor level, and two of them have since then received tenure. Overall, this is part of our strategic work to make our career paths clearer, with more Professors and fewer Researchers, and to include “exit strategies” for those who cannot become professors. This is in agreement with what was recommended to the Chemistry – Ångström department in general by the “KoF 2017” evaluation panel, *i.e.* the UU-wide Quality and Renewal evaluation in 2017. At the same time, we have worked to secure competence and continuity for our research and our education at all levels, including third-cycle teaching and supervision. The Program professor regularly discusses staffing of first- and second-cycle courses with the Director of undergraduate studies and relevant course responsible teachers, and a yearly staffing plan is made. In summary, we have had a significant turnover of senior academic staff, with six of the twelve supervisors in the physical chemistry program being newly recruited since 2012.

The TekNat Faculty has a mentor program for young faculty that several of us has joined as either mentor or mentee. A challenge for new teachers/supervisors from other countries is to master Swedish, to teach many courses at BSc level, be representatives in boards, follow what goes on in the Swedish society, *etc*. As new and non-tenured, there are many other things one must do to become established, and language training often gets low priority. We are discussing and implementing strategies, including setting intermediary goals (such as shorter research presentations in Swedish, the first to be held in December 2020) and offering focused and high-level private language courses.

2.2 Third-cycle program Environment

Assessment criteria:

Research/artistic research at the HEI has sufficient quality and scale for third-cycle education to be carried out at a high scholarly/artistic level and within a good educational framework. Relevant collaboration occurs with the surrounding society, both nationally and internationally.

An international, collaborative environment with critical mass. The group of PhD students with specialization in Physical Chemistry and Chemical Physics is homogenous in age (ca. 23-30 years) but diverse in terms of country of origin: 15 out of 20 (Oct. 2020) were born and took their undergraduate degree outside Sweden. Several of the supervisors have also arrived in Sweden relatively recently. Our working language is thus English. We have a good number of international guest students from undergraduate to third cycle, which includes Erasmus and Fulbright students, as well as free movers. They typically take Master and PhD courses, and do research in collaboration with our PhD students and postdocs. In addition, we have several BSc and MS project students every year, who take part in all group activities. None of our 20 PhD students is making their PhD predominantly outside our department, and we have no industrial PhD students.

All PhD students are employed with salary from day one. We had until recently a few students financed from the Chinese Scholarship Council, who received an economic compensation to reach the same level as a PhD student net salary, according to TekNat Faculty rules.

As usual in the natural sciences, the PhD student conducts his/her research in collaboration with the supervisor, and most often with other junior and senior scientists in the group and/or other research groups and universities. We have research collaborations with leading universities and research institutes in our respective fields that involve our PhD students and lead to joint publications in their theses. This broadens the perspectives and possibilities for the PhD students in terms of shaping their research projects, with access to complementary knowledge, perspective, methods and materials. It helps them obtain national and internationals experience and build networks. In addition, the increased motivation of having a larger group of people directly caring about the details of their work should not be underestimated.

High quality of research. Our environment allows the PhD students to do research at the international forefront. The Department and Research Programs are evaluated regularly. The UU-wide Quality and Renewal ("KoF") evaluation, with an external evaluation panel, has been run 2007, 2011 and 2017. The KoFs have focused on the quality of research in the research programs. Internal TekNat Factulty evaluations were made in 2010 and 2019 to overview the performance of the Programs and their Faculty funding. The third cycle education has been evaluated by UU several times, via surveys (see Section 3.6).

The panel in the UU KoF11 evaluation judged our research to be of "Top-quality", defined as "outstanding work at world leading level with great international impact". This was given to both Physical Chemistry and Chemical Physics programs (this was before we merged the two programs into one, in 2012). Only our programs and Molecular Biomimetics received this grade among the twelve chemistry programs we had at the time. One panel comment was: "Indeed, the program represents the standard against which many efforts around the world are either directly or indirectly compared…[…] …a *significant fraction* of the people involved in this effort represent the very best in the field."

The UU evaluation KoF 2017 concluded for the programs *Physical Chemistry* and *Molecular Biomimetics*: "The panel was impressed by the scientific excellence, the cohesion and the informal collegial culture underpinned by the competent and visionary academic leadership of the program professors. The section is characterised by a positive atmosphere, a culture of scientific excellence, and a strong focus on facilitating innovative research and actively pursuing external funding opportunities. There is a strong team spirit in the section. [….] This culture was underpinned by competent and visionary academic leadership by the senior professors and clearly appreciated by the younger faculty, researchers and research students. [….] On the PhD level, students are given necessary training and are given hands-on access to the advanced equipment of the department. This provides an excellent and unique research training that will give an important competitive advantage to the graduated PhD students."

Our research has received attention in general media in recent years: SVT, Vetenskapsradion (five times), Dagens nyheter, Uppsala Nya Tidning, Aftonbladet, Forskning och Framsteg, and NyTeknik. Our public outreach includes: Scifest (2012-), Teknikåttan, Levande Frågelådan, Augusta Ångström Exhibition, and Solar Days Uppsala. Many of our PhD students take part in these activities.

Collaborations for research and PhD training. We have long-standing and intense interactions with *Molecular Biomimetics* and *Synthetic Molecular Chemistry* research programs. Some students and postdocs have informal or even formal supervisors from these programs. We share many labs, instruments and offices, publish many joint papers and interact on a daily basis. We have one joint coffee/lunch/seminar room, with weekly info-coffee (typically 60 participants), and several joint seminars per month. This is to a large extent an integrated environment between the three research programs, and this significantly increases the pool of PhD students well beyond a "critical mass", and widens the scope, horizon and possibilities for our PhD students. The Edwards group at BMC has similar interactions with *Pharmaceutical Physical Chemistry*. Solar cells research also involves collaborations with *Structural Chemistry*, the Departments of *Physics and Astronomy* and *Electrical Engineering*. Christer Elvingson maintains a collaboration with the Department of *Mathematics*, and joint PhD students partly financed by the School of Interdisciplinary Mathematics. Our collaborations foster cross-disciplinary projects with many joint publications. We also run joint PhD courses (Fluorescence spectroscopy, Semiconductor electrochemistry, Biooorganic chemistry, EPR, Electron transfer).

The most important collaborations and networks for the our *Program* are the Center for Molecular Devices (CMD), the Consortium for Artificial Photosynthesis (CAP), the Phospholipid Research Center, the Centre for Interdisciplinary Mathematics and the Extreme Light Source (ELI). These form a broader scientific "home base" for our PhD students, with collaborations beyond the individual supervisor groups.

CMD carries out world-leading solar cell research with joint effort from UU ((Boschloo, Johansson, Tian, Freitag), KTH and SwereaIVF. A spin-off company, Dyenamo AB, was formed because of the success at CMD. Dyenamo supplies CMD with standard and custom-made materials for solar cell research. CMD and Dyenamo (along with Finnish company Canatu and Aalto University) were granted funding in H2020 (SOLAR-ERA.NET).

CAP (founded in 1994), has been based in Ångström Lab (UU) since 2006. CAP focuses on solar fuels research, and is a world-leading center in the field; international recognition has inspired similar foundations in countries around the world. CAP includes several groups from UU (the Programs of Physical Chemistry, Synthetic Molecular Chemistry and Molecular Biomimetics), KTH and Umeå Univ..

Phospholipid Research Center: The Edward's group has close collaboration with Pharmaceutical Physical Chemistry as well as with Medical Radiation Science (Faculties of Pharmacy and Medicine, respectively) with join projects and equipment, shared PhD supervision, seminars etc. The group is also involved in several international collaborations and is one of the nodes in the global network of researchers in academia and industry that is organized by the German Phospholipid Research Center.

The Centre for Interdisciplinary Mathematics facilitates joint research between the mathematical sciences and other disciplines and industry, and Elvingson carries out research within this centre.

ELI is a new Research Infrastructure of pan-European interest and part of the European ESFRI Roadmap. Sá coordinates the development of an X-ray spectroscopy end station at the Czech Republic site.

EU projects provide important networks and international collaboration. Since 2010, we have been part of four EU projects and six COST networks. We also maintain a joint project with Ghent University in the U4 network. We are involved with several companies, see Section 5.

Seminars. Our joint seminars with external speakers (typically two-three per month) provide scientific breadth, and often include topics related to sustainability, climate and renewable energy, or a recent series on gender mainstreaming (Section 3.5), which put science in perspective of societal questions. All PhD students have to give three formal seminars during their studies, and numerous presentations at group meetings and collaborative platform meetings; sections 3.1-3. They contribute to guaranteeing that the student is ready to defend the thesis.

3. Design, implementation and outcomes

3.1 General aspects.

The Third cycle studies in Chemistry with Specialization in Physical chemistry or Chemical physics comprises 240 credits, of which at least 40 credits is the student's own course work. At least 30 credits of the course work have to be from scientific subject courses (e.g. chemistry or physics but not "Introduction to PhD studies", ethics or pedagogic courses, etc.). A licentiate degree exists, but we have not had a student finishing with a licentiate during the last 15 years, and it is rarely used as an intermediate examination; instead, we have half-time seminars (see next page).

Most PhD students teach, mainly as lab teachers on first or second cycle courses. No PhD student is teaching more than 20% of full time over their studies. A pedagogic course for university teachers (7.5 credits) is obligatory for PhD students who teach.

The formal coupling between learning activities, outcomes and examination goals is controlled in the ISPs, where the Examination Goals are written into the ISP template. The ISP must state what progress has been made towards each goal, and give concrete examples what was done to make that progress, and what is planned to fully reach each goal. Thus, the Examination Goals are broken down in partial goals, and learning activities and outcomes to reach these goals are identified.

It is the joint responsibility of student and supervisor that the PhD training proceeds towards completion within the stipulated time. Some aspects are mainly in the supervisors' control (e.g. lab and instrument access, scientific guidance), other mainly in the control of the student (focus, planning of work hours, etc.). The progress is monitored continuously by the supervisors, who will take action if the situation is not satisfactory. Progress is also monitored via the yearly revisions of the ISP, discussed by the supervisory group, and the formal presentations (four-month and half-time seminars). If progress is slow, and if the formal presentations are not given within reasonable time, the situation is discussed with the FUAP and the supervisory group, and appropriate actions are taken (see e.g. Section 1, page 5).

Increased follow-up activities. On a general level, we have increased the formalized follow-up activities during the recent few years. This originates from discussions at both Department-wide and Program supervisory meetings that were followed by a decision by our Head of Department in 2018. Thus, all new PhD students have to give a short seminar four months after they start, with at least the supervisors and the FUAP present, as well as other students and postdocs in the group. They need to show that they understand the general research topic, its state-of-the-art and key literature. They also have to give a half-time seminar for all researchers in the Program (mandatory attendance). The supervisors and FUAP discuss the seminar, giving feedback to the student (if the FUAP is supervisor, another professor takes that role). Finally, the students have to give a seminar close to their PhD defence, where they practice their defence presentation. They get extensive feedback on both scientific and presentation aspects.

All PhD theses in Physical Chemistry and Chemical Physics are written as summary theses with papers appended. There are no formal rules on number of publications in either UU or TekNat Faculty rules. Quantitative rules will always be blunt, as the variation of student contribution and scientific achievement varies greatly even if "first authorship" or other criteria are used. In practice, our students have at least one "first-author" paper accepted before the thesis is submitted. We also do not think any student during the last ten years have had less than four papers/manuscripts in their thesis.

We have recently (HT 2019) decided that, before the student is allowed to send the thesis to print, the complete thesis has to be read and its content evaluated not only by the supervisors, but also by an independent professor, *i.e.* someone who has not been involved in the research. It would typically be the FUAP, but if the FUAP is supervisor or co-supervisor, this could be a FUAP of a different subject. We believe this is a time-efficient way to increase the quality control.

Area for improvement:

- Evaluation and refinement of the new follow-up activities and recruitment procedures (Section 1).

3.2 Proficiency knowledge and understanding

Assessment criteria:

The programme facilitates, through its design and implementation and ensures through examination that doctoral students who have been awarded their degrees can show broad knowledge and understanding both within their third-cycle subject area and of the scientific methodology/artistic research methodology in the third-cycle subject area.

The formal coupling between learning activities, outcomes and examination goals. Examination of many of the *Examination Goals* is made through the examination of the PhD thesis and the oral defence. As support of this decision is the peer-review process of the thesis papers. A successful publication is a positive *learning outcome* showing that important *goals* have been reached through the *learning activity* of planning, performing, evaluating and communicating research. Additional goals are reached and examined through the PhD courses. Other important and general learning activities and evaluation steps are described below.

The most important activities to promote a broad knowledge and understanding of the subject are third-cycle courses and work on the individual research project. As is typical within natural sciences, the PhD students carry out their PhD research as a series of research projects. Each project is in collaboration with their supervisor(s), often with other group members and other research groups involved. Regular meetings with the supervisors is a most valuable learning activity. "Open-door", *ad hoc* discussions are very common and also very helpful for students to solve the daily problem in lab. Group meetings, where both ongoing research and relevant scientific articles are discussed, are also important to provide scientific depth and perspective. The supervisor and group meetings include methodological discussions, choice of scientific question and the soundness of conclusions drawn etc. in the student's own research as well as in the literature papers chosen.

The research group(s) to which the student belongs is a great source of learning. In addition, our many collaborative projects mean that the PhD students have to explain and discuss their science, and the physical chemistry/chemical physics involved, with researchers from other disciplines, which trains them to communicate their subject in a clear and pedagogic way, and to represent an authority in their discipline.

PhD courses. In order to assure a broad knowledge within physical chemistry (needed also for PhD students in the subject Chemical Physics), which is a necessary outcome independent of whether the future career is in academia or in research and development in industry or authorities, a broad course in *Physical Chemistry* (10 cr) is offered for all PhD students that do not have sufficient breadth and depth from their previous studies. This is not only as a base for the continued progression and specialization; it is also expected that a physical chemist should be able to teach at undergraduate level in all areas of physical chemistry. This requires a broadened and more thorough *understanding*, and not only knowledge about the different areas of physical chemistry. The requirement of at least 40 cr courses in the PhD education also gives a clear progression with a significantly deepened knowledge and understanding within the own specialization. Examples of this can be found in the individual study plans. Examples of more specialized PhD courses we offer to provide learning progression include *Fluorescence spectroscopy*, *Polymer physics* and *Electron transfer*, which all require a prior understanding of *Physical Chemistry.*

A list of PhD courses offered is given on our department web page. As many students benefit from higher-level courses in neighboring subjects (Physics, Mathematics…) the PhD courses listed at the Faculty web page is also highly relevant. TekNat and UU also offer general courses, such as *Introduction to PhD studies*, *Research Ethics* (mandatory), and different pedagogic courses, as well as courses in skills such as academic writing and oral presentation. Some students participate in international summer/winter schools.

In addition, we encourage the PhD students to initiate reading courses in subjects they need to study, in groups with others or individually. One example is the recent *Bioinorganic chemistry* course (see "Doctoral student perspective"). To encourage progression to more advanced and independent studies, we have recently (HT2019) initiated individual studies of topics that are of interest to the individual student and where the student wants to acquire deeper knowledge and understanding. The topic is then presented during joint group meetings, which stimulates thorough command of the topic and helps the learning of others. All PhD students are expected to present one topic per year. The quality of presentations has so far exceeded our expectations, and it is clear that the format has stimulated learning in a good way. We have thus decided to give 1-2 credits for each topic presented. Examples of topics chosen by the student and supervisors include *Transition State Theory, Electronic Energy Transfer* and *Spectral Line Shapes*. The topics presentation are used in the "Friday group meetings" that are joint between five supervisor groups. We have presented the idea and outcome at meetings with all supervisors, and there is an interest in implementing this scheme generally for all our PhD students in the subjects *Physical Chemistry* and *Chemical Physics*. This will be discussed and decided on during the annual follow-up meeting of the Supervisory group (Dec. 2020).

Seminars with invited national and international researchers promote both deeper and broader knowledge of the PhD students. In these seminars, the PhD students learn about frontier research not only in their specific area but also in other areas in physical chemistry and adjacent research areas. We offer on the average about two-three seminars per month during semesters, of which about half are compulsory for our PhD students. The seminars are selected to provide a larger breadth and deeper knowledge of scientific concepts within and behind physical chemistry. PhD students are given opportunities meet the invited speaker after the seminar, during "fika" meetings or lunch meetings to further strengthen scientific interaction and exchange of knowledge between the students and the invited speaker.

All PhD students in physical chemistry are moreover involved in projects connected to at least one school or collaboration platform (cf. Section 2.2). The research platforms Centre for Molecular Devices (CMD) and the Consortium for Artificial Photosynthesis (CAP) include groups from several universities and industry, and this gives the PhD students very good possibilities to meet, discuss and collaborate with other researchers in similar research areas, which significantly contribute to their specific knowledge but also broaden their knowledge and understanding. Similarly, students in the research area Surface, Colloidal and Macromolecular chemistry are part of either the Phospholipid Research Center - the collaborative network with pharmaceutical physical chemistry - or the Centre for Interdisciplinary Mathematics, where they meet students and senior researchers from other disciplines for joint seminars and discussions. Moreover, most students also attend the seminars at the monthly meetings of CAP and CMD. This provides deeper understanding and better contextualization of their research activities. In the recent survey answered by all the 16 PhD candidates in the program, 38% strongly agree and 19% agree somewhat that the obligatory seminar program is important and helpful to develop a broad knowledge, while the rest answer neutral. Our seminar speakers are mostly of good-to-excellent quality. It is important to identify why ca. 40% gave a neutral reply. Are these new students struggling to understand, or cases of seminar fatigue? Are seminars no longer perceived as a good form for transfer of knowledge and ideas, and for discussions? We have discussed this extensively at group meetings and FUAP/student meetings for some years.

In order to further deepen and broaden their knowledge, all PhD students participate in international conferences, typically at least one per year, where they also get the opportunity to present and discuss their research in relation to other international research groups and therefore acquire further specialized and broad knowledge. This also applies for summer/winter schools, which some PhD students attend.

A good test if you really have understood a scientific area is to teach or to give a presentation. The PhD students must give at least three formal oral presentations during their PhD education (Section 3.1). They will receive feedback from the audience in the following discussion, and after the seminar from their main supervisor and the FUAP. There is also a yearly mini-conference for the PhD students at the chemistry section, where they have to give a poster or oral presentation. Moreover, the PhD students have numerous presentations at group meetings and at meetings with their collaborative platforms (CMD, CAP etc.).

Learning progress is achieved by students taking increasingly more advanced and specialized courses, as described above, including the individually chosen topic presentations. They also have to take a gradually increasing responsibility for writing their manuscripts and selecting references, which means that they must fully understand the research field and its state-of-the-art, and for discussing their results and their significance. The oral presentations become progressively demanding, as more advanced content and presentation are expected. Through the feedback they obtain from group meeting presentations, the students improve the way they do their studies, and how they think about and understand them. As they become more familiar with the research of their group members, they are contributing more and more to the discussion of their colleagues' presentations.

In our own survey (Dec. 2019) 75% of the PhD students agreed that the courses and seminars were sufficient to fulfil the Examination Goals of "Broad Knowledge". Only one student disagreed somewhat to the statement that he/she gets enough training to fulfil the goals in the ISP.

Areas for development.

- Evaluate the Physical Chemistry course in its revised form.
- Continuous: identify what courses PhD students lack.
- Analyse and discuss the seminars.

3.3 Competence and skills

Assessment criteria:

The programme facilitates through its design and implementation, and also ensures through examination that doctoral students who have been awarded their degrees can demonstrate the ability to plan and use appropriate methods to conduct research and other qualified (artistic) tasks within predetermined time frames, and in both the national and international context, in speech, in writing and authoritatively, can present and discuss research and research findings in dialogue with the academic community and society in general. Doctoral students are able to contribute to the development of society and support the learning of others within both research and education and in other qualified professional contexts.

The formal coupling between learning activities, outcomes and examination goals on a general level should be ensured via the UU evaluations of third-cycle studies for the six-year cycle 2017-2022 (see Section 3.6). For each Ph.D. student, their progress towards the goals of the Ph.D. education is reported in the yearly revision of their ISPs, which couples learning activities and outcomes to examination and Examination Goals (Section 3.1).

The formal, obligatory seminars after four months and at half-time (Section 3.1) are intermediate check points that the student learning towards the goal progresses in a satisfactory way.

The supervisors and Ph.D. student plan for the writing of the thesis and defense date, and the main supervisor informs the FUAP for approval. If needed, this may lead to a thorough discussion of the student's progress. When the student is about to defend, a preliminary internal assessment of the thesis is done by the FUAP to guarantee that relevant goals of the research education have been achieved (see Section 3.1).

To ensure that students are also prepared to meet the quality standards of the oral presentation of their thesis defence they are requested to give a test presentation in front of their supervisors and their research group or/and as a part of divisional seminars. At this presentation, they are to discuss the science with authority, with a synthetic understanding of their work and that of others, and to discuss future directions. The program has established routines that provide the student with detailed feedback in oral and written form, from the general audience and specifically assigned members of their research group that addresses content and layout of their presentation and their presentation technique.

The student's ability to conduct their tasks within a predetermined time frame is guaranteed by the four-year (full) time frame of the PhD studies, and where our average time is 4.37 years (Section 3.5). Intermediate Goals also have to be met in time: scheduled formal presentations at the department and at international conferences; time goals are set for paper writing; teaching has to be prepared in time, etc.

Learning progress is achieved by students taking a gradually increasing responsibility for planning and evaluating their research, and for communicating the results in scientific papers. The later papers build on the outcome of the previous ones, which provides progression in subject learning. It gives a possibility to go deeper into the scientific questions, and critically discuss their previous publications. The level to which this occurs depends naturally on the individual student and on the project.

Moreover, presentations at group meetings and other meetings are reoccurring, and through the feedback they obtain, the students improve the way they do their studies, and how they think about and understand them. The formal presentation put progressively increasing demands on the student, from the four-month presentation were an overview of the research field and scientific questions, with key references should be given, via the halftime presentation where the student's own results should be presented and discussed with some authority and in an international context, all the way to the final presentation. In the latter presentation, and during the defence, they should be able to discuss with greater authority, and be able to discuss knowledge synthetically, and discuss future directions. They also get to present to a wider audience at collaborative platform meetings and international conferences, with increasing demands on cross-disciplinary communication, promoting the learning of others, and presentation with authority. As they become more familiar with the research of their group members, they are contributing more and more to the discussion of their colleagues' presentations.

For the learning of others, progression is also achieved regarding undergraduate teaching: the PhD students often start by teaching large lab courses in collaboration with a more experienced lab teacher. In later years, they may help younger colleagues instead, and are responsible for more advanced lab experiments, and often co-supervise BSc and MS student projects or visiting student projects. Important and general learning activities are described below.

Learning activities. At our program, we have established a range of measures and routines that enable and make sure that the PhD students reach the goals of the research education and acquire skills and abilities to plan and perform high quality research and other work that is relevant both in academia and in an industrial setting.

Interaction with supervisors and peers. A particularly important instrument of the Ph.D. education at the program is the intensive interaction with the supervisors including regular and comprehensive feedback given to the students in oral and written form. For this purpose, in all research groups at the program there are regular meetings (typically every other week) where students discuss individually with their supervisor the advancement of their research project. It is primarily *via* this interaction with the supervisor that students acquire the necessary skills and abilities to plan and perform scientific research in a progressively independent way. At the same time, these meetings enable supervisors to monitor the student's progress towards the specific goals of the Ph.D education and scientific autonomy in general and identify issues and needs in this process. A formal assessment of the student's progress is provided on a regular basis in form of written feedback from the supervisors in the yearly revisions of the individual study plan (ISP). Our recent survey (Dec. 2019) including all Ph.D. students in the programs showed that the feedback they get from their supervisors is among the most valuable contributions of the program to support their development.

The research group(s) to which the student belongs is a great source of learning. New students learn methods and experimental techniques from a more senior student or postdoc, and sometimes even collaborate on a first project. Conversely, more experienced students get experience from instruction new PhD and Master students and thereby in supporting the learning of others.

Training in presentations. All students write several scientific papers and a summary thesis. The work to identify and plan for a potential paper, all the way to finally publishing it, is repeated during the PhD training. This provides good training in planning and executing advanced research within a given time frame and in being able to present and discuss the results with authority, in written form. Progression is achieved by a successively increasing degree in student independence in that process.

Corresponding training in oral presentations and discussion is given. All students at the program participate in conferences in Sweden and abroad, contributing with their own posters or oral presentations. The conferences cover a very wide range of topics where Physical Chemistry is relevant, as e.g. spectroscopy/photochemistry, renewable energy, materials science and technology, drug delivery etc. and are often of multi-disciplinary character. Attending typically at least one major conference per year, the students progressively develop their ability to present and discuss their findings in discourse with experts in their field as well as a broader scientific audience. As a result, students improve their communication skills, obtain critical and inspiring input on their research and broaden their perspective on their field of research and the subject area in general. Presentations for the respective research group, or as part of divisional seminars or seminars in conjunction with other departments, schools or research platforms described previously, provide the students with plenty of opportunities to progressively develop the skills and abilities required for major conferences and their doctoral defense. At groups meetings and halftime seminars, we give formalized feedback not only on the scientific content but also on the quality of presentation. According to our recent survey (Dec. 2019) conducted with the Ph.D. students, these exercises, together with the opportunity to attend conferences, are very valuable for their development. To support and promote attendance to these conferences, there are funds available from different sources (department, faculty, student nations, etc.) All students at the program apply for and obtain e.g. the Liljewalch's Resestipendium, ÅForsk travel grant and Wenner-Gren travel grant. Liljewalch's is in practice guaranteed when the student has reached 2 years since admission). We are also not aware of a student that has not been able to go to any conference during years 1-2 because of lack of funding.

*External seminars***.** During their Ph.D. studies, students at the program have also the opportunity to interact closely with well-known visiting researchers in their respective areas. We organize several seminars with international researchers (ca. 2 per month during a semester). In addition to our regular seminars, all PhD students have the opportunity to select and invite one internationally well-known researcher for a seminar and 2-3 days visit, to build contacts to other research groups in the world. The student is responsible for arranging the visitor's program, including interactive lunches and dinners, and for keeping the budget. This seminar should ideally be about one year before the student defends, when the student has reached a level of maturity and will start planning for the future. It requires of the student to be able to identify an interesting guest, and provides insight into the academic culture of exchange visits and how to organize scientific interactions. These visits have been very valuable for the student and the entire environment. Not all PhD students make use of this opportunity, and their number has unfortunately decreased in recent years. During 2021, we will investigate the reason for this and discuss with the current students how to encourage this activity when the pandemic so allows.

Support of the learning of others; contribution to development of society. Most of the Ph.D. students in the program are involved to a significant extent (typically 10-20% of full time) in teaching of undergraduate students. This is mostly as lab instructors, in some cases also leading seminars or problem solving classes. PhD students participate in preparing laboratory instruction material and are responsible for the practical instruction of students, and the assessment of their lab reports. As lab instructors, they also convey knowledge of proper use of equipment including laboratory safety. All students that teach have to take a pedagogic training course (7.5 cr). Another requirement is participation in an introductory course for lab teachers (two full days). During their teaching, the new PhD students are also coached with respect to teaching methods and practical matters by the course responsible and senior teachers in the same course.

Most teaching is done in Swedish, in particular the larger courses during BSc level years 1-2, with many lab groups. This has meant that teaching has been unevenly distributed. Some Swedish-speaking students have felt they get too much teaching (never above 20%, however), while some students who do not speak Swedish have complained that they are not able to teach. Over recent years, we have therefore increased the practice of English-speaking lab teachers also on bachelor level years 1-2. The bachelor student groups have viewed this as mainly neutral or even positive, according to course evaluations. Many of our PhD students are also involved in the supervision of Bachelor and Master Student examination projects, and projects of visiting students. These are done in English, and is another opportunity for all PhD students to practice supervision and contribute to the learning of others. In the Department alumni survey 2018, 74.5% replied that they had taken part in at least some training for PhD students/teachers. It has recently become clear that many PhD students do not know the "rules" for how the teaching is counted as work time. These are mostly straightforward and the same as at most Swedish Chemistry departments and our Department is communicating these rules to all PhD students.

Because of the group composition and international diversity, our working language is English. We offer possibilities for Swedish (and English) language courses, paid by the Department, and recently via free courses from the Department of Nordic Languages, but only some PhD students make the effort. It is also hard to practice speaking Swedish at the department when English is the dominating language. Still, Swedish is needed at courses, in department boards etc., and is important for a work life in Sweden after the PhD degree.

Outreach. To develop students' ability to communicate their research also to the general public, the program provides various opportunities to participate in outreach activities that are regularly mentioned in the local and national media. PhD students from the programme have e.g. been involved with Sci-Fest, an annual three-day event since 2014, and the Ångström laboratory's 20 years anniversary (2017) with demonstrations and practical activities for the general public in relation to solar energy research carried out at the program. They were also actively involved in the development of a solar cell kit for high school students ("Skolceller") in collaboration with TekNat samverkan. Schools can borrow these boxes with instructions to make their own dye-sensitized solar cells in the classroom. PhD students are encouraged to engage in outreach, and many teachers/researchers are engaged, but we offer no formal incentive to do so.

Areas for improvement:

- Encourage foreign PhD students to learn Swedish.
- Increase the number of students who take the opportunity to invite an external speaker.
- Communicate to the PhD students how teaching time is counted.

3.4 Judgement and approach

Assessment criteria:

The programme facilitates through its design and implementation, and also ensures through examination that doctoral students who have been awarded their degrees can demonstrate intellectual autonomy, (artistic integrity), and scientific probity/disciplinary rectitude as well as the ability to make assessments of research ethics. The doctoral student also has a broader understanding of the science's capabilities and limitations, its role in society and human responsibility for how it is used.

Students begin their PhD program with a structured discussion of their individual study plan (ISP); judgement and approach in the context of research and science is one component of the ISP. The ISP contains examination goals that evaluate the student's ability to independently carry out research science with – regarding *Judgement and Approach* – specific attention paid to these *six criteria*: *i*) intellectual autonomy, *ii*) scientific integrity, *iii*) research ethics, *iv*) perceiving the possibilities and limitations of research, *v*) awareness of the role of research in society, and *vi*) the responsibility of the individual for how research is used. Progression in judgment and approach is fostered by many activities that are inherent to the PhD program in physical chemistry; several types of regularly occurring activities that encourage such development are described below.

Progression is achieved not only by increasingly difficult tasks, but also because repeated reading and writing makes progression: a beginner does not have the same perspective as a mature student, and is not able to pick up the same issues. A mature student is expected to write a much more complete draft of higher quality than that of an early stage student. Ultimately, a good judgement and approach should be demonstrated through the thesis and defence, in the discussion of the student's own results, how they are interpreted and put in relation to the work of others.

Ethics course. A 2 cr ethics course is compulsory for PhD students at the TekNat Faculty, and our students take a course arranged by the TekNat Faculty.

Formal research presentations. Students will prepare and give many research presentations while in the program. The formal presentations at four months, halftime and shortly before the defence (see above) are some of them. The PhD students also participate in weekly/biweekly group meetings where they either give a presentation or provide feedback on presentations by other group members. These meetings provide a format for independent critical thinking and analysis of their own research (presenter) and peer review (meeting participants). The PhD students participate in schools or research platforms where they will share their research with a larger group of peers. In this context, the role of science in society is discussed as it relates to e.g. energy, climate and sustainability. They also participate in international conferences, where societal aspects are often included in the presentations and discussion.

Giving and observing research presentations is training on the *six criteria i-vi* above. Intellectual autonomy is practiced when students prepare scientific presentations for coherence and insight. Scientific integrity and research ethics are practiced when students give honest and fair reporting of data and analysis of results; this is both in one-on-one meetings with the supervisor and in presentations to collaboration partners and ant group meetings. Presentations are also one format where students motivate the positive and potentially negative societal impacts and limitations of scientific contributions made by their research.

Participation in seminars, lecture series, and courses. Seminars, lecture series, and courses that support PhD student growth regarding the *six criteria i-vi* are held on a regular basis. Students in physical chemistry are obliged to attend weekly departmental seminars where national and international guest speakers present cutting edge research. In these seminars students can gauge the impact of others' research on society, practice the peer review of research taking place outside of their department, and discover how other researchers handle ethical aspects of research. In their 3rd or 4th year, each student is encouraged to select and host an international seminar speaker (Section 3.3), which requires a high degree of intellectual autonomy. We invite external speakers with expertise in the areas of science that impact energy, climate change and sustainability. This broadens the PhD student perspective beyond what is regularly encountered in the department. Physical chemistry students must participate in lecture and seminar courses to meet their 40 credit degree requirement. In seminar courses, students must read, critically analyze and, discuss scientific literature. Importantly students need to clearly: identify what assertions authors make, judge the strength of those arguments based on the evidence (data) provided, and assess the value of the research to science and society. Skills regarding *criteria i-vi* are practiced in this process.

Discussions of current literature often leads to ethical questions: what data and analysis justify the claims? How is data (not) presented? Are the citations appropriate and balanced? This is discussed at group meetings and informal literature clubs. Writing their own papers leads to similar questions, which are discussed with the supervisors and other co-authors.

Experimental execution. In order to obtain a PhD in physical chemistry, most student need to perform their own experiments that involve the use of chemicals. From this perspective students need to consider the ethics and environmental impact of their own (and others) research on a daily basis. Risk assessments are used to ensure responsible handling of chemicals and equipment. The risk assessment also encourages students to replace toxic and or dangerous chemicals with safer alternatives whenever possible. The risk assessment thus engages students in *criteria i-iii*, and *vi*. Experiments give rise to data; when students analyze and communicate their findings and conclusions into presentations and written communications (vide infra) they practice their ability to work independently in the lab, their scientific reasoning and ethics, and perceive the possibilities and limitations of their research.

Written communication of research results. PhD students must communicate their scientific achievements to the broader scientific community by preparing manuscripts for publication in peer reviewed journals and writing a thesis. These activities build their intellectual independence, research ethics and integrity, while the peer review process tests their scientific reasoning, possibilities and limitations of their research by those outside the department. Taking charge of the peer review process by, for example, responding to referee comments further develops their intellectual autonomy. Finally, by publishing their research, students need to consider the implications of how their research may be used by others.

Formal and informal discussions. Since spring 2019, the FUAP calls to a half-day meeting with all PhD students in the subjects *Physical Chemistry* and *Chemical Physics*. One intention with these meetings is to discuss issues regarding *judgement and approach* with all students. Thus, the agenda has so far included discussions on student/supervisor responsibilities in different situations, as well as plagiarism and self-plagiarism. During formal annual discussions with supervisors, students review and update their respective ISP. Students track their progression in their PhD education and assess themselves on *criteria i-vi* above; this process gives awareness of the importance of judgement and approach in their education. Students also are encouraged to define the direction of their own research, which develops their autonomy. For example, according to our anonymous survey (Dec. 2019) of the 16 PhD students in physical chemistry/chemical physics, 75% of the students are confident that they can perform their research with autonomy. The majority of the remaining 25% did not feel confident or unconfident in their autonomy and one student did not feel that they could perform research independently (note that the students were from beginners to their 4th year). Informal discussions about the ethics and global implications of research (mis)conduct, sustainability, climate change, etc. take place in the coffee room and at group meetings. They are often initiated by recent events reported in e.g. the media. PhD students engage to varying degrees in those discussions. The yearly FUAP meeting with the PhD students gives us one opportunity to make sure that all students are involved in such discussions. Our anonymous survey (Dec. 2019) revealed that 100% of students feel that they perform their research to the highest ethical standards.

3.5 Gender equality

Assessment criteria:

A gender-equality perspective is taken into account, communicated and supported by the content, design and implementation of the programme.

The physical chemistry program (to which all PhD students in *Physical Chemistry* and *Chemical Physics* belong) contains individuals with different gender identity, social background, ethnicity, abilities, disabilities and age. The view on gender equality is affected by previous experiences and social background of the individuals. To gain democratic participation and change social problems connected to gender inequality, a *dialog* with all employees concerning gender equality insecurities are highly important. Based on the individual's experience we can thereby make visible new perspectives and see points where further development on gender equality are necessary. At our Department, we have identified the Program professors as of importance for identifying possible strategies to improve gender equality. Therefore, the equal opportunities group together with a gender specialist from the HR office at Uppsala University are performing deep interviews to understand the possibilities and challenges the programs have concerning gender equality. This is a long-term work aiming at gender mainstreaming. It is during decision-making that unconscious bias concerning gender has the most severe impact. At the faculty level, we have taken measures to improve our meeting cultures, by performing meeting observation with equality as focus. This is a strategy we would like to introduce to our program, since it has shown to be efficient.

In our anonymous survey (Dec. 2019) we asked PhD students from the physical chemistry program whether they thought that the atmosphere at the workplace encourages an open dialogue about gender equality and gender-related issues. The underlying aim with the survey was to gain knowledge of the status concerning gender-related issues of the PhD students, but also to indirectly create an awareness and develop a dialog about gender equality. A majority of students agreed that our workplace encourages an open dialogue. This is not surprising, as some members of physical chemistry program have organized a gender mainstreaming initiative in the department (gender mainstreaming means integrating a gender equality perspective at all stages and levels of our work and activities). Starting in 2019 and continuing now, Dr. Glover and PhD student Sigrid Berglund (both from the physical chemistry program), are hosting focused talks from visiting lecturers and group discussions surrounding the issues of gender mainstreaming in the Department of Chemistry – Ångström Laboratory. The gender mainstreaming initiative is funded by UU to sponsor gender equality works. We also note that it seems to be normal, within our program and at the Department in general, also for research leaders/supervisors to take significant parental leave. At TekNat Faculty, PhD students are allowed up to three months increased study time if they have taken at least four months parental leave. Support for Assistant professors taking parental leave is also given. Our PhD students were also asked (survey Dec. 2019) if they perceived that the workplace strives for gender equality on all levels of employment. A majority of students agreed that the physical chemistry program was working toward gender equality, while three students did not see it that way.

The gender distribution of PhD students in Physical Chemistry and Chemical Physics was according to the survey 7/8/1 (male/female/non-binary; 10 f/ 9 m in Sept 2020); for postdocs the distribution is 6 m/7 f.; Researchers 1 f, 1 m; Full prof 1 f, 3 m; Assoc. prof: 1 f, 4 m, Assist. prof.: 2 f, 0 m. As seen from these numbers, the physical chemistry program has progressively fewer underrepresented genders with higher levels of employment. This is a common situation in academia, but the physical chemistry program is currently acting to further gender equality at all levels of employment. This is a process that has to be continuously developed by creating an inclusive environment. As an example, the Department and Program are supporting the Assistant Professors with one PhD student each to strive for retention of the underrepresented gender. Furthermore, the Equal Opportunity Group for Kemi-Å is continually working towards implementing new strategies to improve gender equality at senior levels of employments. Such strategies will also be implemented in the physical chemistry program. One example, in addition to retention, is recruitments where we may announce (assistant/associate) professor positions in areas where there are strong female candidates.

Further challenges are to actively remind e.g. PhD students about university gender equality policy and how to act in case of incidents. This includes informing whom to contact, rights and obligations in case of incidents. Leading actors within gender equality questions will give a voice to them whose voices are not heard or listened to. Furthermore, it is important to look over the setup for group meetings, who is talking and why? Who is listened to and why? How are responsibilities divided up and based on what background? The department and the physical chemistry program are striving for a gender balance in all the commission setups, dealing with program matters and decisions. However, in a program as ours with few female faculty members it is not easy to live up to the 40/60% in all boards and commissions since it might be negative for the individuals. Therefore, to not overload women with commissions, we need to make sure that the women will be represented mainly within the groups where the most important decisions are taken.

The Physical Chemistry program professor has taken an active role in understanding and informing about sexual harassments and how such matters should be dealt with. Printed information (in English) regarding harassment is put on the coffee room notice boards. All employees and visiting researchers are given information on equal opportunity during their introduction with our HR, including rules, policies and support around harassments. One recent improvement (in progress) is that they have to hand in a signed reply to a quiz on this topic to the program professor for approval (similar to what we do for lab safety with undergraduate students). The idea is that this should guarantee that the information reaches everyone with at least some degree of attention.

As is common at Swedish universities, our UU and TekNat faculty rules stipulated until this year that all PhD thesis committees have at least one female and one male participant (a binary perspective). Since this year, our new rules state instead that committee members should represent different genders (a non-binary perspective). Recruitment and search committees and evaluators for positions must be selected including both binary genders, and must consider gender aspects in the evaluation process.

Areas for development: Persistent work is needed on most aspects of this criterion. Specifically:

- Improve gender balance on the professor level.
- Follow-up on gender mainstreaming and anti-harassment initiatives.
- Improve gender balance among External Examiners and seminar speakers.

3.6 Follow-up, measures and feedback

Assessment criteria:

The content, design, implementation and examinations are systematically followed up. The outcomes of the follow-up are translated, when necessary, into measures for quality improvement, and feedback is given to relevant stakeholders.

The HEI works for the doctoral student to carry out the programme within the planned period of study.

The organization and responsibilities for third-cycle education were described in Section 1. Both UU and the TekNat faculty carry out regular evaluations of the third-cycle education. The organization is set up for systematic evaluation of quality and progress. The UU Vice Chancellor has decided on a model for evaluations of third-cycle education with “sharp” evaluations every six years (e.g. via UKÄ, or otherwise via use of external evaluators) and continuous follow-up with research evaluations and surveys. In addition, there must me a yearly report from each Department to the TekNat Faculty Board. During the six-year cycle 2017-2022 the yearly report must include eleven aspects defined by the Vice Chancellor.

On the individual student level, the most important tools are the ISP, the supervisor meetings after revisions, and the formal presentations, as described in several sections above. Below we describe the systematic evaluations on the level of the *Physical Chemistry* and *Chemical Physics* subjects as well as on the TekNat Faculty and UU level.

The TekNat Faculty organizes yearly meetings for all FUAPs and Directors of third-cycle studies. These include current information, and focus on spreading good examples of increasing PhD education quality. Questions regarding quality and processes are discussed, often identified in the yearly reports and follow-up of third-cycle studies, and in the future from the “sharp” evaluations during 2020-2021. Information is relayed from FUAP to supervisors and PhD students.

The Faculty Board for third-cycle studies (FUN), where teachers from all sections are included, meet three to four times per semester to discuss joint topics and issues on third-cycle studies, and to prepare discussions and decisions before Faculty Board meetings.

On department level, the Director of third-cycle studies call all supervisors to meetings once per semester, where we discuss current and general issues. In the Physical Chemistry Research Programme, the *Supervisory group* (Section 3.1) is an important forum, For example, the increased follow-up activities with obligatory four-month and half-time presentations were discussed on both lunch meetings and the yearly formal meeting, before we decided, *i.e.* the increased level of structured follow-up is a result of feedback from and discussions among the supervisors. FUAP gives feedback to the PhD students.

The yearly meeting of all PhD students with the FUAP was started in 2019 as way to increase the direct contact between FUAP and all students in a systematic way, to improve possibilities for feedback from all students, and to be able to communicate important points, discuss with and give advice to all students. The students are requested to give feedback and suggestions on the conditions for their third-cycle studies. This is then communicated by the FUAP to the supervisor and others concerned, in a suitable manner. Important changes we have made in response to this feedback include the reshaping of the broad PhD course in Physical Chemistry (see below) and the clarifications and updates of instrument responsibilities, which are now also found on a joint server area.

The individual PhD students are requested to give feedback in the ISP revisions. They are welcome to give feedback at any time, via their supervisors, FUAP, Director of third-cycle studies or Head of Department.

Research evaluations: The department and research programs are evaluated regularly with respect to the quality of our research and the research environment, which are important also for the PhD education. UU has conducted three large evaluations of all research, the Quality and Renewal evaluation (KoF 2007, KoF 2011 and KoF 2017; see Section 2.2). The KoF 2017 panel report notes: "On the PhD level, students are given necessary training and are given hands-on access to the advanced equipment of the department. This provides an excellent and unique research training that will give an important competitive advantage to the graduated PhD students." The panel noted, however, a general criticism of lack of career planning on most levels. This has initiated a discussion on how to implement that also on the level of PhD training. (see more in Sections 4-5 on the resulting activities).

Third-cycle evaluations. The UU unit for Quality and Evaluations is regularly evaluating third-cycle education via e.g. survey studies. The most recent one for TekNat was conducted in 2015, and the responders were PhD students (658 individuals), alumni (560 individuals) and supervisors (568 individuals). In all three groups, 55-58% responded. The report was presented in January 2017 together with written reflections on the results from each Department, with the aim to identify areas for development and demonstrate good examples.

Positive aspects from the students in the 2017 report were possibilities for independent work and development, and the availability of good supervisors. On the negative side was that many were uncertain of the demands and what was expected from them, and many were unaware of the examination goals. A large fraction among both supervisors and students did not find the ISP helpful in planning and following up progress. In response to this, the TekNat faculty and our department has improved the IPS template, and developed a structure where plans, activities, examination and progress towards the Examination Goals are clear. Our previous Director for third-cycle studies has given presentations and courses for FUAPs, supervisors and PhD students on how to write the ISP.

Nevertheless, we who write this self-evaluation feel that the ISPs have improved greatly over the years. There is a clear connection to the Examination Goals of the activities, learning outcomes, examination and intermediate goals. This forces both student and supervisor to think and realise what they are already doing towards the Examination Goals, and what additional activities etc. that needs to be planned. This is a strong improvement that is implemented partly in response to the results of the survey and report 2017, and to the many discussions within TekNat. What may be perceived as a weakness of the ISPs is that the research is not described in a way that allows a third-party evaluation of its quality. This would require a quite extensive and detailed research plan, which would require some time to write, and it would then become a public document. For the purpose of this UKÄ evaluation, the summary nature of the scientific projects is of no concern, however, as this aspect is not being evaluated.

Alumini surveys. The UU unit for Quality and Evaluations and our Department have conducted several surveys among alumni on a third cycle level, as described in Section 5. In 2018, our Department surveyed 125 former PhD students in all specializations from the previous ten years (51 replied). Most of them were satisfied (66%) or mainly satisfied (30%) with their education, and 92% would have chosen to do a PhD if they could choose again. Interestingly, only 35% of the respondents were aware of the Higher Education Goals. This shows that our work to include these goals explicitly in the ISP (see above), which had already started, was important.

Course evaluations. Our Master program on Chemistry was evaluated by UKÄ in 2013, and the outcome was very positive ("high quality"). The evaluation committee concluded that the strong research and its international reputation permeates the whole master programme in chemistry and is also an important reason for recruitment. The programme further prepares the students well for their future career. This was also confirmed by our alumni survey. The high quality is important here because we recruit PhD students from that program, and the PhD students often take advanced courses from the Master level. The courses on the Master Programme are systematically evaluated. The evaluations are used on a Department level and on a Faculty level by the Educational Program Boards ("Programråd") to monitor quality. Feedback is given when needed to the department and teacher responsible for the course, and there are frequent requests for improvement, and sometimes greater changes are made and courses are even replaced.

The PhD courses are evaluated mainly via direct discussions with the students. Frequently, the courses and teaching are planned together with the students, and changes can be made as the course progresses. One recent example is the discussion during the Fluorescence Spectroscopy course (2019, *ca.* 10 participants) on the way the seminar discussions was conducted and how to distribute the word more equally. Another recent example is from the spring 2020 FUAP meeting with all PhD students, where we discussed the broad course in physical chemistry (15 cr). The frank and constructive criticism from the students has made us reshape the course entirely, and it is given in a new format starting October 2020.

Average time for third-cycle studies. During 2012-2019 among 103 students at Kemi – Ångström, the average study time was 5.63 calendar years, while the average effective (full) time was 4.37 years. While this is somewhat higher than the stipulated four years, it is a typical figure within TekNat, and we do not think this is an important problem. Some positive actions have contributed to a longer average study time, such as the possibility of up to three months increased study time if the student has taken at least four months parental leave. We have only had one dropout student during the last 15 years. We have had other students during the same time who have had severe difficulties, but that we have been able to help so that that they finish a PhD, often a very good one! In general, these students have not needed more time than the average. Our conclusions are that many students are at risk of getting stuck, being trapped in negative circles and/or experience unhealthy and unproductive stress. Regular supervisor meetings and systematic follow-ups are important to identify and alleviate problems as early as possible. Strong coaching can make such a student rise far above his/her expectations, and in most cases make them successful. Nevertheless, there are limits of what supervisors and all our measures to secure a supporting environment can do for an individual. In some cases, the best outcome is then if the students terminated their studies, preferably with a licentiate degree, if they have reached the corresponding goals.

***Area for Development*:**

- Systematic collection and documentation of all the Department's PhD course evaluations is being planned by our Director of PhD studies.

Reflections on the ISPs. Our anecdotal impression from many meetings and conversations at TekNat over the years is that many supervisors and students have been uncertain what the purpose of the ISP really is. This impression seems to be supported by the result of the 2017 report. At least initially, many regarded it as a planning tool for the research project and courses of the PhD student. While this was an understandable purpose, many felt it was unnecessary to fill in all details that both supervisor and student thought were obvious, e.g. taking part in group meetings and seminars. Then for some years, authorities gave the impression that the IPS is mainly a legal document between the department, supervisors and the student, to be used in case of conflict. The more recent interpretation, in line with the present UKÄ evaluation, is that it is indeed a tool for planning and follow-up, but that it should also be used by third parties for quality control. This caused strong reactions from many supervisors at TekNat, and they argued that the IPSs were not written for that purpose and could therefore not be used for a fair assessment of the education. The uncertain and shifting perception of the purpose of the ISP has not been beneficial for their quality. It is also seen in the rather important differences in the ISP template requested at TekNat, and how differently the ISPs have been written over just the last five years.

4. Doctoral student perspective

Assessment criteria:

Doctoral students are given the opportunity to take an active role in the work to improve the content and implementation of the programme.

The programme ensures a good physical and psycho-social work environment for the doctoral student.

How PhD students can influence their third-cycle studies. UU, TekNat faculty and our Department are regularly making investigations and surveys involving active PhD students and alumni, as described in the previous sections. This is an important way that PhD students can influence the third-cycle studies in a broader and perhaps longer time perspective.

For the preparation of this UKÄ self-evaluation, the views of Ph.D. students were collected via an anonymous survey (December 2019) including all 16 PhD students in *Physical chemistry* and *Chemical physics*. Two volunteer PhD students read the entire evaluation and made suggestions that were implemented. According to the survey, 13 of the 16 doctoral students in the programs feel that they are in control of the direction of their research, which is in complement to the high degree of student autonomy in the physical chemistry program. This control manifests itself in many areas of the program.

The Department Board always must have a least two doctoral student members (and two working Substitutes). They have a particular responsibility to gather information and opinions from PhD students to the board, and to report back to the students. Each year elections are held by students to elect the student members to the chemistry board, thus giving students an active role in the decision-making in the Chemistry Program. PhD students also have representatives in the Faculty PhD Council (“Doktorandråd”), in the Faculty Board and its Board for third-cycle studies (FUN).

The yearly meetings between all PhD students and the FUAP is another important opportunity for the students to shape their PhD program. Informal exchange of opinions and suggestions is also encouraged.

Student influence on their own particular studies.

The students have large influence over their own studies, and freedom to access all our labs and equipment (following proper training). In their research projects, the student will be progressively more knowledgeable and mature to suggest new ideas and research angles, and the freedom to do so is relatively large in most cases. We keep the research plans of the initial ISP (at admission) rather open and general, because we want the student to be active in shaping his/her own project. The first steps of doing so occur in parallel to the preparation of the four-month seminar, and the ISP is updated shortly afterwards. Among the more senior PhD students, several collaboration projects have been initiated by the students.

Students are encouraged to organize their own courses when they see a need it to augment their research. In 2019-2020 academic year two students from the physical chemistry program organized and participated in a 10 credit *Bioinorganic Chemistry Course* to further their understanding of metals in biology.

Students at the program also have the possibility to suggest and/or decide conferences, workshops, etc. they would wish to attend, taking thus an active role on the profile of their education. They are encouraged to suggest invited seminar speakers. We also have a program where all students are allowed to select and invite one internationally well-known researcher for a seminar and 2-3 days visit (see Section 3.3).

The yearly revisions of the ISPs includes the view and reflections of the Ph.D. students concerning the role of their supervisors, the quality of the supervision, and whether the goals of the research education are being fulfilled satisfactorily. The students thus participate actively in the evaluation and future planning of their education.

The opinion on the level of independence that a student should have varies greatly between PhD students, as well as between students and supervisors. The question on responsibilities and independence has been taken up in discussions (group exercises) in the yearly meetings with all PhD students and the FUAP.

Work environment. We provide a mentally and physically healthy work environment for our PhD students, with channels for PhD to express their viewpoints and suggestions for improvements. In our own survey among PhD students (Dec. 2019) a majority said they feel that they work in a mutually respectful and inclusive environment. Respect and inclusivity is the foundation of a mentally healthy work environment. The PhD students are invited to a yearly half-day meeting with the FUAP, to which they are asked to bring up topics of concern or discussion and to give their views and opinions. Work environment issues (physical work environment, stress, conflicts etc.) should also be part of the yearly ISP revisions.

In our own survey (Dec 2019), the students also agreed to a very high extent that their supervisors are scientifically very competent and have sufficient pedagogic competence to work well as supervisors. They thought that they get sufficient supervision time, and that it is easy to get more time if they need. These aspects are important for a positive work environment for the PhD students.

Every three-four years a Department work environment survey is given to all employees, coordinated by UU centrally, and the last two times they were performed by the company Quicksearch. In the most recent one (2020), the physical chemistry employees listed Job satisfaction, Respect, Appreciation and Inclusion as strong aspects. The general work climate was perceived as very good. Our overall index was equal to those of the best sectors in the country (e.g. IT sector). The somewhat weaker sides were "work-life balance" and "clear expectations with reasonable conditions" (64% and 68% score, respectively, where >70% is good), but it was mainly Professors/Researchers who gave lower scores. The majority of doctoral students feel that they work in a mutually respectful and inclusive environment, according to the survey. This is an important aspect of a healthy work environment. We strive to maintain good physical working conditions. For example, students have the right to meet with an ergonomic specialist to optimize their workspace; this can include getting a standing desk and/or ergonomic office chair. All departments at Ångström lab have grown, and the campus is finally expanded with new buildings to allow us more lab and office space during 2021. We also take laboratory safety very seriously. Each student (and lab worker) is trained in laboratory safety where proper handling of chemicals and waste disposal are a part of the training. Since 2018 a “Risk Assessment” must accompany all experiments involving chemicals. The written document is just one of many measures that ensure a safe work environment.

During the covid-19 pandemic, we have discussed transparently at open zoom meetings how to handle the work situation, and how to work in safe way, being respectful of others. Clear information has been given by UU. Web-based meeting and teaching tools have been expanded rapidly. We already had good web-based library resources. Working from home when possible has been encouraged. Considering the general circumstances in society, it has worked well, but of course it is both a practical and a mental burden, and more so for some individuals. Like everywhere in academia, employees including PhD students have made extra efforts to make things work, showing great loyalty to their work, their colleagues and the undergraduate students. UU and TekNat has included a brief form as an appendix to the ISP revision in this October, where each PhD student should report how the pandemic has affected their doctoral studies and how much time has been lost. A complete overview of the effects is not available, but preliminarily it seems that our PhD students have typically not lost less than one month each and in the worst cases three months.

Point of reflection: On point of concern is that students are often financed by external grants, so if the project direction changes, alternative financing may have to be arranged. It is a general weakness in the Swedish financing system for research and third cycle education that a large part of research and PhD education is expected to be financed by external grants tied to a very specific project (ca. 75% at our TekNat faculty). This significantly limits the scientific freedom of PhD students. Yet, few if any PhD students complain about this, and most of them are actively seeking to work in the particular project. It is worth discussing if the present system *is* a problem, and if the scientific independence of the students would be improved if their project funding were completely open.

Area of improvement: More office- and labspace when we move into a new floor at Ångström (2021)

5. Working life and collaboration

Assessment criteria:

The programme is designed and implemented in such a way that it is useful and develops doctoral students’ preparedness to meet changes in working life, both within and beyond academia.

In order to grow and to be prepared to meet work life challenges in and out of academia a person needs to have acquired certain skills. Communication, problem solving, critical and creative thinking, self-learning, collaborating, short and long-term planning, organizing and executing, and self-reflection are highly valued skills. Not only are these skills relevant in a day-to-day context, but one’s career and most certainly in earning a PhD. Our PhD program not only reinforces these skills, but also necessitates that students hone and improve them.

Subject-specific skills from the PhD program are transferrable to the job market.

Communication. To act as a productive member of any workplace, one must not only do the work that is needed, but also communicate the outcome of that work. In previous sections we have touched on how students improve their communication within our PhD program, but it is clear that the ways in which PhD students practice the communication of their science will be useful in their future careers. Written, oral and visual means of communication are inherent the work of the PhD program. Participation in conferences, regular group meetings, teaching, and outreach events are all examples of how our PhD students practice communicating visually and orally to peers in their field and the general public. Written communication is practiced to a very high degree when students write up their findings for publication in scientific journals and in the preparation of their thesis. Student's abilities in written communication nearly always improve as a result of their PhD studies. The improvement in all forms of communication is indispensable for any future career PhD students embark upon.

Lead and instruct others. The role of teaching has been discussed above in terms of meeting the goals in the PhD program (Section 3.3). When students teach within their field of expertise several things happen that are useful for their professional working lives: *i)* As teachers, PhD students are leaders of the classroom, as such they gain valuable leadership experience, *ii*) A large proportion of our students also share in the supervision of Bachelor and Master Thesis work, which trains their skills in leadership and supervision. *iii)* The act of teaching trains students to adapt to a dynamic work environment where what is needed of them may change from moment to moment, *iv)* Teaching is a way for students to practice ways to communicate difficult and/or abstract concepts to those who have less knowledge than them. *v*) Significant *planning* must occur prior to stepping into a teaching laboratory or classroom. Designing the lesson plan, or the protocol for laboratory experiments, requires that student teachers *plan* well ahead of time (*adhering to timeframes*). In all, while having teaching experience is a sought-out merit for jobs in academia or teaching in high school, teaching also improves many skills that are broadly useful in working life.

Successfully completing advanced tasks while adhering to timeframes is a transferrable skill in any workplace. Carrying out research in a chemistry laboratory is not intuitive and the use of certain chemicals and instruments is inherently dangerous. Lab work also involves a significant amount of *planning* prior to setting foot into the lab. Experimental work can be a complex process and at times stress-inducing. Under such conditions, students must also learn how to work independently, with accuracy, precision, and safety in the laboratory to produce results of high quality and without bringing harm to themselves and others. Effective laboratory work takes years of practice. Skills involved in lab work are directly transferrable to many jobs in chemistry. Should students not take up careers where laboratory work is required, learning to succeed in a difficult task while under pressure is a transferrable skill in any workplace. As a majority of laboratory work is independent, PhD students also increase their self-sufficiency as a result.

Advancement of intellectual skill. A natural outcome of PhD research is that students push the boundaries of knowledge and technology. When PhD students carry out research in physical chemistry, they will produce data for the chemical system they study, and then need to interpret the data to explain microscopic events that are not visible to the eye. This will invariably require the skills of critical thinking, problem solving, and self-learning. A corollary to this is that students must weigh how to handle and report their data in an ethical manner. We have described how our students are trained in ethics in Section 3.4, and with respect to student led advancement of knowledge by performing research, they put their ethics into practice. During the PhD studies, such skills will be applied mostly in the context of physical chemistry. Critical thinking, problem solving, being able to learn on one's own, and responsibly using and reporting data are skills that are still useful in careers inside and outside academia, as well as in every day life. Advancing these intellectual skills during PhD prepares students to independently tackle challenging tasks in their future careers.

Collaborations. PhD collaboration opens possibilities future career steps. In professional work environments, it is routine to work as a team to achieve a common goal, i.e. collaborate. Research is not a solo venture for a PhD student; minimally the student will work with their advisor. All PhD students in the Physical Chemistry Program engage in some form of collaboration which can take place within the Physical Chemistry Section, in the Chemistry Department, with other Departments at Uppsala University, other universities, and with groups outside of academia. Such collaboration can be tracked in the peer reviewed publications authored by our PhD students.

The program of *Physical Chemistry* has close contacts with other groups/departments at Uppsala University and is active in several broader research platforms (Section 2.2). PhD student participation includes giving professional presentations, sharing the workload involved in interdisciplinary research projects. Several of the research groups have close contacts and collaborations with research institutes within Sweden, for example SWERIM, and IVF Swerea. Also, the physical chemistry program has been instrumental in the spinning out of three companies: Nuclisome, Dyenamo AB and Peafowl Solar Power AB. These three companies along with Fresenius Kabi and AstraZeneca are examples of non-academic players that some PhD students from our program have interacted with.

Outside of Uppsala University, PhD students have participated in collaboration with groups from international universities, e.g. Yale University, Rice University, CalTech, University of Chapel Hill, Texas A&M (USA); Cinvestav (Mexico); Tsinghua University, Beihang University (China); Masdar Institute-Khalifa University (UAE); Sungkyunkwan University (South Korea); University of Nantes (France); Aalto University (Finland), EPFL (Switzerland); Cambridge University, Imperial College London (UK); Ghent University (Belgium); DTU (Denmark); Lund University, KTH, Stockholm University (SE), to name a few. Collaborations outside of Uppsala University benefit PhD students by building up their professional network, and can sometimes lead to students landing their next job after earning their PhD degree. For example, three former PhD students and one postdoc have been employed by SWERIM over the last 10 years. Also, within the last three years two former PhD students have been employed at Imperial College London as postdocs with our collaboration partner in the EU SUN2CHEM. International collaboration further broadens the PhD student perspective, on international groups and their research. Finally, when students engage in collaboration, they can experience comradery and mutual respect for fellow researchers, which can be positively motivating.

PhD student responsibility beyond their individual research. As members of a shared laboratory space, PhD students in physical chemistry are delegated responsibilities to keep the lab running smoothly. For example, one rotating lab position is the ordering of chemicals and consumables needed for the research group. PhD students all share the responsibility to keep the laboratory workspace clean and free from hazards. Most students take the responsibility to maintain an instrument and train the new users who wish to use them. Taking on such duties strengthen teamwork and camaraderie among the PhD students, which is a necessary skill in all workplaces. Further, many students from the Physical Chemistry Section have taken up positions on University boards e.g. the Chemistry Board and the Equal Opportunities Board. These appointments are important to ensure that student interests are represented in decisions taken at the Department and University levels. When students participate in these boards they gain experience thinking beyond their own interest to make decisions that affect their entire cohort, which is something that is relevant in working life in an out of academia.

Work life beyond the PhD. In our own PhD student survey (Dec. 2019), 69% strongly agreed and 19% agreed somewhat that the competences and skills acquired during their PhD prepares them for the job market in the academia. 44% of students agreed totally or partially that it prepares them for a job *outside academia*. Based on this feedback, it was clear to us that we have room to improve. We realize that from our perspective as academic supervisors, we are in many ways not the most qualified to give career advice for jobs outside of academics. Further, while the annual revision of the individual study plans typically include discussion relevant to the PhD's future working life, we have not applied a systematic approach among all the supervisors. Below we describe how we are taking action to improve students' readiness for jobs outside of academia.

Grant writing. One skill in which academic supervisors *are* qualified to advise is grant writing. The ability to attract funding is key for students that wish to pursue a career as a researcher both in and out of academia.

Grant writing can appear in many other careers as well. Thus, we believe it's important that the students get to practice writing applications for travel and research grants. To this end, the PhD students usually apply for funding, both internally (e.g. Liljewalch's scholarship) and externally (e.g. ÅForsk travel grant), for travelling to conferences during their PhD. Furthermore, we have begun to organize a yearly workshop for application writing and evaluation, with the first one taking place in February 2020. The students are given the opportunity to assess anonymous grant applications submitted to the national or EU agencies (generously shared by the authors), which had different success outcomes. They are provided similar instructions to the ones given to evaluators. Student then evaluate these grants in a discussion panel; this exercise gives students insight into how to effectively convey new research ideas and avoid pitfalls when eventually applying for their own funding.

The alumni perspective. The UU unit for Quality and Evaluations has conducted two larger surveys among alumni on a third cycle level (2006 and 2015). The TekNat alumni were asked in what way that different component of their PhD education have been useful. 85% of the respondents said that they were very or rather satisfied with their PhD education at UU, and 88% were employed within three months after finishing their PhD studies. For PhDs in Physical Chemistry and Chemical Physics, we estimate that about 50% get jobs in industry, research institutes, public agencies or similar. About 40% take up postdoctoral research, mostly facilitated by obtaining individual grants. Some study pedagogics and become high-school teachers.

We are not aware of anyone during the last 20 years who was unemployed for longer than one year after earning their PhD degree, and in most cases they were employed much sooner than that. We realize that we lack clear and systematic data on the employment and careers of our PhDs once they have left the Department. Thus far, alumni surveys suffer from poor response rates. A further complication is that many former PhD students are difficult to track down, especially if they have left Sweden. One point of improvement is to compile the information we have and fill in the gaps (in accordance with GDPR rules). Increasing the amount of feedback from our alumni will help us understand how we can better serve our students moving forward.

Student and alumni mixers. In order to bring students the perspective of what faces them after the PhD it is perhaps best to let the experienced tell their story. In previous years PhD students organized alumni evenings, with one-two former PhD students presenting their work and their perspective on their PhD education. All current and former physical chemistry teachers, staff, postdocs and PhD students were invited to meet, eat and mingle. These were enjoyable evenings of reunion and opportunity for informal networking and asking questions. Since ca. 2011, this activity ebbed out. We have now been able to rekindle such events in the department. Presently we have asked that two current PhD students to organize each event to take place once or twice per year. This is an important way for the students to influence their education, get career advice and insight, and network with alumni in other sectors. We think it empowers our students to share the responsibility for these evenings. One evening was planned for April 2020, but was postponed due to covid-19. A simpler, zoom-based talk of one alumnus with Q&A was held on Nov 17, 2020, and one is planned for the spring. For now we will continue to hold these a zoom-based meet-ups until it is safe to hold physical meetings.

Career Days. Currently, neither the Physical Chemistry Program nor the Department organizes any institutionalized career days. However, we successfully lobbied the PhDs to include company representatives in the Chemistry Mini-Conference which is held annually and organized by PhD students in the Chemistry programs. Thus, in the 2019 Chemistry Mini-Conference included two company representatives (GE and ÅF), two gave talks and all three visited the stands during the poster session. The students invited a guest speaker to discuss a career change from research in chemistry to gender research. According to the final survey, the large majority of the students enjoyed this activity, which they aim to repeat in future PhD in Chemistry Mini-Conferences. The 2019 conference was attended by 37.5% of the Physical Chemistry PhD students. We will continue to encourage participation of all Physical Chemistry PhD students.

Areas for development:

- Career planning, alumni contacts and career days.
- Mapping of PhD alumni employments and career (preferably on Department level)
- Structured career discussions during renewal of ISP.