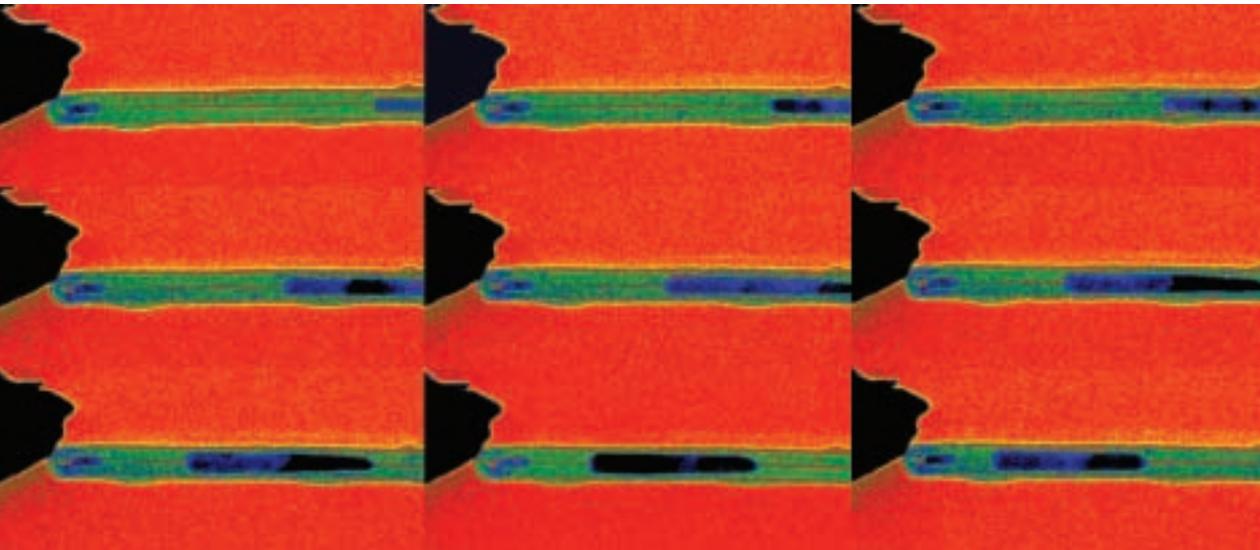




Vetenskapsrådet

## EVALUATION OF THE SWEDISH CONDENSED MATTER PHYSICS, 2004



International Evaluation of

**SWEDISH CONDENSED**

**MATTER PHYSICS, 2004**

EVALUATION OF THE SWEDISH CONDENSED MATTER PHYSICS, 2004

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Vetenskapsrådet

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Cover Photo: Sequential TEM images of an iron filled carbon nanotube (40 nm in diameter) subjected to a high electrical current density, causing electromigration of iron in the direction of the electron flow.

Courtesy: Krister Svensson, Eva Olsson (CTH), and Håkan Olin (Mid Sweden University).

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## To the Swedish Research Council

The Council for Natural and Engineering Sciences (NT) at the Swedish Research Council (VR) decided early in 2004 to evaluate the research within Swedish Condensed Matter Physics. A panel\* of international experts was appointed in April 2004, with a Swedish chairperson as well as a Swedish secretary. The expert panel was provided with written reports by the research groups and divisions in Sweden working within the area. Site visits took place during December 2–10, 2004. During this time, the groups under review presented their research activities to the panel.

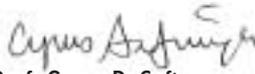
The present document reports the findings and recommendations of the expert panel. By signing, the international experts take full responsibility for the scientific judgements, and related issues, in this report. The chairperson and the secretary confirm that the work was conducted in accordance with the statutes of the Swedish Research Council and that it was performed in an impartial manner.

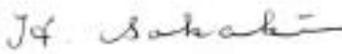
July, 2005

  
Prof. Anne Borg

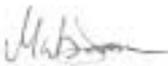
  
Prof. Yvan Bruynseraede

  
Prof. Talat S. Rahman

  
Prof. Cyrus R. Safinya

  
Prof. Hiroyuki Sakaki

  
Prof. D. Phil Woodruff

  
Prof. Mats Larsson

  
Dr. Joakim Amorim

Chairperson

Secretary

\* *Reservation: Prof. Ian Affleck*

A seventh international expert was included in the panel, but chose not to sign the report:

*"I resigned from this committee because I was not satisfied that it would produce unbiased and accurate relative ratings of the 50 or so groups and 150 or so grant holders in Swedish Condensed Matter Physics. Having a relatively large committee doesn't necessarily make this daunting task easier if they can't agree on a uniform rating scheme. I intend to submit a brief report of my own, after the committee report is published."*



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# EXECUTIVE SUMMARY

Overall, condensed matter physics research in Sweden is in a very healthy state. Both the quality and quantity of research are far higher than one might expect for a country with the small population of Sweden, and the only other countries in a broadly similar situation, which might compare favourably with Sweden, are the Netherlands and Switzerland. The Expert Panel found many excellent and world-leading activities within the groups they reviewed, and no research, which was not worthy of support.

While in a country with the size of Sweden it is inevitable that the depth of coverage of all areas of condensed matter physics varies, the breadth of coverage is large and the community has responded to new and emerging fields of interest. In general, the infrastructure of national research resources is very good, with the provision of synchrotron radiation at MAX-lab being an outstanding aspect of this infrastructure, which does much to underpin the very high quality of research in surface and interface science, and related electronic spectroscopies. There is a very substantial and successful effort in the relatively new subject of nanoscience, and the traditional strength of theoretical condensed matter physics in Sweden continues to underpin experimental work across the whole field. There is also a very significant level of applied research interfacing fundamental studies to industrial development and commercial exploitation.

This extremely favourable situation, however, appears to be under threat by the unusual nature of the interface between universities and the funding agencies in Sweden, which has led to a large fraction of university researchers, in nominally “permanent” academic positions, who rely in large part on research income for their own salaries. It appears that this is having an adverse effect on the scientific ambitions of many aspects of future research plans, and could also have a devastating effect on many individuals if, through the changing priorities of Swedish research funding initiatives from agencies other than the Swedish Research Council, such as the SSF, Swedish Foundation for Strategic Research, the level of funding of condensed matter physics research were to be reduced.

# GENERAL RECOMMENDATIONS

## University Positions

1. The poor employment security for researchers with, in principle, permanent positions is perhaps the most serious problem in Swedish condensed matter physics. Faculty positions funded by “soft money” from a number of short-term contracts have created a very unstable situation, which puts the individual researchers under severe pressure and makes it virtually impossible to embark on long-term, risky, projects. This problem must be solved by a concerted effort involving the Swedish Research Council, other funding agencies, the universities, and the Ministry of Education, Research and Culture. In particular, we *recommend* i) that in the future, universities should not make commitments to “permanent” positions, which cannot be fully underwritten by university funding, and that such positions should not rely, in the long term, on external funding; ii) that government funding of universities be increased with the specific objective of guaranteeing the salaries of a larger number of faculty staff engaged in condensed matter physics research; iii) that clear agreements between the Universities and the Research Councils be established over the issue of overheads to ensure that the full net value of grants is used for the intended purpose (such as research student scholarships or salaries).
2. The gender balance in Swedish condensed matter physics is not healthy. The insecure career structure is probably one important factor, which may be affecting young women more adversely than men in similar situation. This is covered in point 1 (*above*). The Expert Panel *recommends* the Swedish Research Council to set aside funds that will allow researchers to re-enter their careers after sustained periods of parental leave.

## Research Activities

3. The present environment for high-risk projects in condensed matter physics is not very healthy, which to a large extent is linked to point 1. When the employment security situation has been improved or solved, the Expert Panel *recommends* that the Research Council launch high-risk projects in basic condensed matter physics by means of a bottom-up approach.

4. Condensed matter physics in Sweden contains a significant component of applied research, and it is very obvious that this is a direct result of the pressure on researchers to go applied in order to stay funded. Whereas the Expert Panel does not have a mandate to make suggestions to other funding agencies, it encourages the Research Council to adhere to its mandate to support basic research (some of which may underpin applied work).
5. The Expert Panel feels that the condensed matter physics community would be well served by a national meeting occurring on a regular basis. The Condensed Matter Physics Section of the Swedish Physical Society could, for example, organise these meetings. The Panel also encourages the Swedish condensed matter physics community to increase its national collaboration.
6. The Expert Panel *recommends* that expensive equipment, clean rooms, and other high-price items be concentrated in those places where they can best serve as user facilities.

## Funding and Management Strategy

7. It is surprising and unsatisfactory that applications submitted to the Swedish Research Council, and the award of grants by the Research Council, appears to incur no formal involvement of the central University authorities in relation to strategic planning or to the contractual relationship, such as the level of overheads to be charged to a contract. This has contributed to the tenuously-funded position of many academics, and to research being under-resourced because overheads larger than those explicitly awarded by the Research Council are deducted by the university or the department. The Expert Panel *recommends* that applications be signed also by a designated university official, reporting directly to the university president, and that such signature guarantees no overheads other than those previously agreed with the Research Council are deducted from the amount received by the researcher.
8. The Expert Panel *recommends* more pronounced strategic planning at all levels of the research system – department, university, funding agency, the Ministry of Education, Research and Culture; and communication between these parts.
9. The Expert Panel *recommends* that the Research Council consider allocating larger amounts of funding for scientific equipment, in particular medium-expensive equipment, where the current level of funding is quite low.

10. There is a danger that the total funding for condensed matter physics in Sweden may decrease in the future as a result of various recent decisions: for example, reductions from the the Research Council's Energy Committee and reductions from the materials science programmes from the SSF. Unless immediate action is taken, some very high-quality research could be down-sized or even terminated. The Expert Panel *recommends* that the Swedish Research Council allocate part of increased Government funding during the next three years to condensed matter physics to compensate for the foreseeable future cuts.

# INTRODUCTION

Condensed Matter Physics (CMP) is the largest area of physics research, in Sweden as well as worldwide. The field accounted for about 40% of Swedish physics in 1992, according to the *International Evaluation of Swedish Physics* (the former Swedish Natural Science Research Council (NFR), April 1992). Since 1992, condensed matter physics, defined in a broad sense, has increased significantly in Sweden, whereas other areas of physics have remained constant or may even have decreased. The reason for the expansion is that new funding sources, in particular the Swedish Foundation for Strategic Research (SSF) and the EU framework thematic programmes, have become available to researchers in condensed matter physics, but to a much lesser degree to researchers in other fields of physics. Condensed matter physicists also had a stronger presence in the former Swedish Research Council for Engineering Sciences (TFR) than other physicists. When the new Swedish Research Council was formed (in January, 2001), condensed matter physics, including semiconductor physics, materials physics, and some engineering physics (i.e., the review panel O and parts of review panels L, P, and Q, which to a large extent contain CMP research) comprised significantly more than 50% of the support to physics and, roughly, more than 15% of the total support to the natural and engineering sciences. These figures depend, of course, on how narrow or broad is the definition of CMP. However, it is obvious that the high volume of condensed matter physics in Sweden has had consequences for the work of the Expert Panel. It was not possible to carry out an evaluation of individual research projects, and the level of evaluation has instead been chosen to be that of research groups (or divisions). In most cases, this turned out to be a practical level, but even with this reduction of evaluated entities from about 170 grant holders to about 65 research groups, the scale of the evaluation far exceeds that of other recent international evaluations, such as those of Meteorology (March 2004, 23 projects) and Biotechnology (April 2003, 32 projects). Since the Expert Panel made site visits to all the major universities except Umeå, and heard presentations from all research groups at the major universities, including Umeå, it is obvious that the Panel was confronted with a daunting task. A few research groups covered in the present report certainly fall on the borderline of condensed matter physics, but have been included in order to illuminate the border region.

The increase of Swedish condensed matter physics can be illustrated using the statistics from 1992 as reference point. In 1992, 217 physicists with

a Ph.D. were working in condensed matter physics in Sweden, whereas the number in 2004 was 417, i.e., an increase of about 90%. The present evaluation probably applies a somewhat broader definition of condensed matter physics than that used in 1992, but even after correcting for this, the increase is still large, of the order of 80%. Similar numbers are found when comparing the number of active Ph.D. students in 1992 and 2004, namely an increase from 259 to 418.

The expansion of condensed matter physics has consequences, some positive, and some negative. On the positive side, the Expert Panel notices, with some surprise, that the infrastructure has not been lagging behind. On the contrary, the research groups are generally well equipped. It is clear that the Knut & Alice Wallenberg Foundation has played a key role in keeping the expanding condensed matter physics community at the cutting edge in terms of infrastructure. Important advances in synchrotron radiation facilities at MAX-lab, namely the construction and commissioning of MAX II and several undulator-based beamlines, have also been a significant positive factor. It is also gratifying to note that the high quality of the scientists has been maintained during this expansion. One reason for this is that the expansion took place during a time when many first rate scientists from the former Soviet Union became available to universities in the West. This has made the expansion possible without compromising the quality of Swedish condensed matter physics, which in general is highly competitive internationally.

On the negative side, it is very obvious that the university system has not been able to accommodate the large expansion. Out of the more than 400 Ph.D. scientists active in the field, only about 10% have faculty positions fully funded by the universities and with full tenure. This problem is addressed in a separate section of this report (“Employment structure, the 25 – 50% professor and the university – research council interface”). The unstable situation, potentially disastrous if funding were to diminish, is causing nervousness in the community, which pervaded all the site visits. In some presentations, long-term vision was lacking, and the focus was on how to survive beyond the end of the contract period.

This organic, rather than strategic, expansion has taken place with the tacit consent of departmental and university authorities to the highest executive levels, yet the full implications do not appear to have been considered. In a period of expansion, this has worked very well and produced several outstanding research groups, and in general, a very high scientific level of condensed matter physics, with essentially no weak groups. However, it is clear that the expansion cannot continue, and indeed, it is likely that a reduction in the total funding of condensed matter physics from all agencies

in Sweden will occur in the future. During the expansion period, soft money entry was the normal way to recruit new faculty. The Panel learned from the executive level at Chalmers University of Technology that much stricter rules would be implemented, beginning in 2005. Other universities are likely to follow Chalmers's example.

# GENERAL ISSUES

In this report, the nature and quality of the scientific research being conducted with the Swedish Research Council support, by individuals and groups within Sweden, are described in a series of sections devoted to specific topic areas. There are, however, a number of more general aspects of the organisation and practice of condensed matter physics within Sweden, and its funding, which are common to all these topics areas. These more general areas are described in the beginning of this section.

## Employment Structure, the 25 – 50% Professor and the University – Research Council Interface

As in other countries, the government is funding scientific research carried out at Swedish universities through a dual support mechanism: direct funding of the universities, which is particularly relevant to salaries of faculty members, and research grants allocated to specific projects by the Research Councils. In other countries, the funding to the universities guarantees the full salaries of faculty members (although in the United States, this is often deemed to cover only nine months of the year; the faculty members are then able to use research grants to cover the remaining three months (the summer period) if they so wish). Research grants provide funds for scholarships or salaries of Ph.D. students, fixed-term postdoctoral researchers, equipment, and general running costs. In Sweden, however, research grants, such as those allocated by the Swedish Research Council, can also be used to pay part of the salaries of the faculty members. As far as the members of the Expert Panel are aware, this situation is unique worldwide.

In the last decade or so, this research grant funding structure has led to a huge expansion in the number of university researchers who nominally have “permanent” faculty positions, but whose salaries heavily rely on continuous research funding. In principle, faculty members who fail to gain sufficient research funding to cover the necessary component of their salaries can increase their teaching commitment and gain a larger fraction of funding from the university. In practice, the amount of teaching time and associated funding is much too small to allow a significant number of faculty members to rely on this fallback position. Typically, the number of faculty members

in the departments associated with condensed matter physics is two to four times that of those who can be fully supported by their universities. At a time of expanding research funding, this high level of commitment is sustainable. At a time of contracting funding, the situation is unstable and many faculty members who have employment contracts which appear to give them permanency, are likely to lose their employments.

In this context, it is interesting to contrast the present situation with the concerns of the members of the 1992 review of the whole of Swedish Physics regarding the career structure for academic researchers. The problem identified at that time was labelled “the missing Associate Professor”, and referred to that fact that there was then no method for lecturers to be promoted to professors, thus making it impossible for excellent researchers to progress through the academic ranks in a natural way. Since 1992, this particular problem has been addressed – and this promotion route does still exist, while the initial distinction, which was made between appointed and promoted professors, seems to be slowly removed. Unfortunately, the situation, which now exists, particularly in the area of condensed matter physics, is even more serious. Younger researchers can be appointed to faculty posts and may be promoted, but do not have the employment security associated with such positions in other countries.

The most obvious consequence of this state of affairs is the unsatisfactory personal situation which many such faculty staff find themselves in, particularly at a time of falling success rates in gaining research funding. This is partly due to a reduction in the available funds, and partly to increased demand (exacerbated by the increasing number of institutions making a call on these funds). In the words of one outstandingly able young academic, whom the Panel met, these people feel as though they are “sitting on dynamite”. Many people recruited from outside Sweden had no idea that this problem existed when they accepted their positions.

Apart from this problem of staff insecurity, however, there are several other negative consequences of this situation, which impact on the whole future of condensed matter physics research in Sweden. For example, several faculty staff members relying on support from the Research Council for their salaries have told the Panel that they

- are now focusing on applications to the Research Council for their own salaries and not applying for support for a Ph.D. student or post-doctoral salaries – this is likely to lead to a reduced number of young scientists entering the field;
- have little enthusiasm to undertake adventurous or exploratory work, which may not guarantee the flow of publications that underpins the next research grant proposal;

- have difficulty in developing and seeing through a long-term coherent research strategy, in part because building up the resources and skills may lead to similar periods of lower productivity in terms of published papers and peer recognition, and in part because trying to ensure that new grant proposals are funded encourages researchers to follow current fashions rather than long-term programmes. Indeed, this sometimes also encourages a “buck-shot” approach to grant proposals, in which researchers may initiate a series of quite different simultaneous activities to achieve adequate salary funding.

The Panel also identified other problems in the interface in the university/research council dual support mechanism, which are having a negative impact on the research conducted. Specifically,

- although the Research Council awards a 35% overhead on research grants, the universities typically take a larger component of the money awarded for this purpose, and in some cases significantly more. The researcher is thus left with a shortfall in, for example, the salary or scholarship for a research student;
- apart from this overhead issue, the actual cost of a research student varies from institution to institution, mainly because in the technical universities students are invariably put on a taxable salary immediately, while in some other institutions the first two years are funded by a scholarship, which is exempted from salary tax (in Swedish “utbildningsbidrag”). Coincidentally, the normal practice in many other European countries is to use non-taxable scholarships (e.g., limited to four years) throughout the Ph.D. period. The net effect of the practice in Sweden is that the total cost of funding a research student is much higher than elsewhere, although most of the extra money goes back to the government, which is funding the student;
- the appointment of faculty members through “soft money” from the Research Councils, particularly for individual fellowships, has meant that University departments appear to have grown in an unstructured way – with little evidence of strategic planning of the research structure of the department. Indeed, the fact that applications for funding, and contractual acceptance of funding, involves only the department and not the central university administration, means that the universities as a whole have no direct input into these strategic issues at the time that initial commitments are entered into.

It should, perhaps, be remarked that the large expansion of high quality condensed matter physics research in the last decade has been a very

positive outcome of the partial funding of faculty positions by the Research Councils. However, the fact that much of this funding has been a result of targeted funding in materials science by the SSF, which is not expected to continue at past levels, clearly means that the present situation is not sustainable without a significant change in future funding. A stable system in the future is only possible if there is a significant reduction in the number of faculty members or if new money is found to guarantee the salaries of many of the existing staff. Reductions in the numbers of faculty positions with the present funding could be very severe and would have a strong negative impact of the high level of excellent condensed matter physics research currently going on in Sweden. The alternative is that new government money is put into the universities to guarantee faculty staff salaries. In principle, of course, another solution is to have “permanent” researchers funded by the Research Councils embedded in the universities as, e.g., occurs in France through funding by the CNRS. This would, of course, necessitate a significant increase in Research Council funding. It would also cause a major change in the structure of research in Swedish universities and divorce teaching from research, both of which the Expert Panel views as undesirable.

The Panel therefore *recommends*

1. that in the future, universities should not make commitments to “permanent” positions that cannot be fully underwritten by university funding, and that such positions should not rely, in the long term, on external funding;
2. that government funding of universities be increased with the specific objective of guaranteeing the salaries of a larger number of faculty staff engaged in condensed matter physics research;
3. that clear agreements between the Universities and the Research Councils be established over the issue of overheads to ensure that the full net value of grants is used for the intended purpose (such as research student scholarships or salaries).

## Inbreeding and Recruitment

In the 1986 evaluation of Swedish Condensed Matter Physics (by the NFR), the Evaluation Committee expressed concern regarding inbreeding in this field in Sweden. Currently, the situation is quite different at most institutions. Today, the evaluated groups in general have researchers of a number of nationalities. A major reason for this change is the large expansion in the field in Sweden over the last years, in part made possible through hiring

of highly qualified researchers from abroad on soft money, including a number of highly competent people from Eastern Europe. However, in the case of Swedish researchers in the field, it remains true that there has been limited mobility between the different institutions. Hiring of people at the new universities is an exception. For a young Swedish researcher returning to Sweden from a postdoctoral period abroad, it is easier to seek funding through collaboration with his/her former research group in Sweden, than through collaboration with research groups at other Swedish institutions. Continued recruitment through soft money is not expected to change this situation or to contribute to the mobility among the universities. In addition, while the new research career structure, implemented in 1999, allows lecturers to be promoted to professors, this does not encourage researchers to seek professor positions and research opportunities at other Swedish institutions.

To promote mobility among the Swedish universities and assure recruitment of excellent candidates in the future, the Expert Panel *recommends* public announcement of vacant, permanent positions at the professor and lecturer level. These positions should be announced internationally. In addition to attracting a larger number of highly qualified candidates for the available positions, such a recruitment policy will allow the institutions to develop and impose their research strategies. Permanent scientific staff below professor level at different institutions should therefore have the opportunity to apply for announced professorships at other institutions as well as seeking promotion at their home institution through the newly introduced promotion system.

## Women in Condensed Matter Physics in Sweden

During its site visits to the different condensed matter physics groups, the Expert Panel noted a low number of female presenters, in particular among the permanent scientific staff. From the numbers made available from the Swedish Research Council, the number of female researchers is 33 as compared to 284 male researchers (postdocs not included) in the area of condensed matter physics, according to the broad definition of CMP covered by the evaluation.

Recent numbers presented by the Swedish delegation at the IUPAP International Conference on Women in Physics, Paris 2002, showed that about 30% of the graduate students in physics in Sweden at that time were women, while the corresponding number of professors was about 7%. The

number of female graduate students does not differ very much from the number of female undergraduate physics students.

Sweden has clear gender equality policies, a well-established child care system and 16 months parental leave, of which about 13 months are at 80% salary, for each child. Ph.D. students automatically have their scholarship period extended to account for parental leave. In the Swedish Research Council, they already apply a policy of taking into account parental leave when evaluating applications. In this respect, the opportunities for women to make careers in science as well as in other areas are very good. Over a number of years, the government has provided several initiatives to promote opportunities for women to make careers in science, including the 32 “Tham Professors”, specially allocated for women. The Research Council has also experimented with special researcher positions for women in engineering science (six positions in the year 2003).

Despite these clear positive policies, there is still a considerable “leak in the pipeline” in terms of females seeking an academic career in science in general, and in physics in particular. In Sweden, as in the other European countries, the critical point in the career is after the candidates have finished their graduate studies. At this point, the candidates are expected to spend a period as postdocs abroad, before returning to Sweden. After returning from one or several postdoc positions abroad, the next step on the career ladder is to apply for a time-limited position as research associate. Not many are successful, at this point, in the present funding situation in Sweden. In addition, there is no guarantee that there will be a permanent position available at a university after finishing a period as research associate even after doing well scientifically during this period. Furthermore, it should be noted that one is not eligible for a fully paid parental leave if one has not had a paid work for at least six months within the last twelve-month period in Sweden. This is an extra complication for candidates pursuing a scientific career, because of the pressure to spend postdoc periods working abroad. As the path to a scientific career is highly uncertain, in a period of life where many are having children, it is not very attractive to young researchers, and in particular, not to the female ones.

Changing the number of female scientists in the area of physics, as well as in other areas of science, is not a simple task, but it should be addressed. In Sweden, the Swedish Research Council, together with the Ministry of Education, Research and Culture, and the universities, should consider strategies to overcome the lack of clear career paths in physics. Clearer career strategies may make it more attractive for women to seek a scientific career; and more attractive to the women after finishing graduate studies.

The Expert Panel suggests some possible initiatives, among which, one is selected as a general recommendation in this report:

1. Establish “post-parental-leave grants”, which could consist of one- or two-year grants for researchers after sustained parental leave. This could provide an opportunity for researchers to re-enter the scientific career.
2. Establish three-year postdoc positions, the last year of which can be spent in Sweden for re-entry to the Swedish research community following a period as a postdoc abroad. In this way, some of the uncertainties, regarding both parental leave and having an employment to come back to in Sweden for a limited time, could be reduced.
3. Establish postdoc positions, which allow for a combination of short-term periods abroad with periods at a Swedish institution; in this case an institution other than that from which the candidate has graduated, in order to promote mobility inside Sweden.
4. Offer research associate positions allocated for female applicants. Such positions could make it more attractive for women to seek an academic carrier.

In addition to the measures taken by the Research Council, a possible action at the university level could be to provide fellowships to female physicists at the associate professor level. Fellowships could be provided for reducing their teaching load, hiring a postdoc or in other ways supporting their activity, in order to give them enhanced opportunities to qualify for promoted (or full) professorships. This fellowship should last for at least one year, preferably longer.

## Balance in the Field

### Basic vs. Applied Research

One striking feature of the material presented to the Expert Panel, both in a written form and during the site visits, was the significant component of research which was of a relatively applied character or which had clear links to future applications. Of course, condensed matter physics does have strong direct ties to materials applications, but in Sweden, applied science has separate funding agencies, e.g., SSF, VINNOVA, and STEM. Therefore, one might have expected that the amount the Research Council-funded work directed to applications might be rather less than in other countries, whereas the general impression was that there was significantly more. While it was clear that there was a widespread perception that gaining

funding was more likely to be successful with an applied bias in the work, it was not really clear where this pressure came from, at least for the Research Council-funding. Significant amounts of the Research Council-funded work with no very direct applications, particularly in theoretical physics, clearly showed that funding could be achieved with such a programme. On the other hand, many of the largest and best-funded groups clearly benefited from access to a multiplicity of funding agencies, including not only the Research Council and the SSF, but also VINNOVA and the European Commission. To benefit from this range of agencies, a significant applied element in the research programme is essential, and it is possible that this is part of the underlying motivation. One might suggest – with such a range of alternative agencies – that the Research Council-funding is not important, and should be directed elsewhere. However, there are clear examples in Sweden of outstanding research programmes with strong applied research funding for which modest funding by the Research Council underpins their ability to bid for these additional funds. Nevertheless, one conclusion of the Expert Panel is that it is important that the Research Council continues to fund core work in basic condensed matter physics, both theoretical and experimental, without the need to stress any short or mid-term perceived application.

## Experiment vs. Theory

An important aspect of Swedish condensed matter physics has been the close collaborative effort in theory and experiment in many subfields and in most institutions, which has worked to the advantage of both; and placed Sweden as one of the pinnacles of learning and discovery in the area. Not surprisingly, Sweden has produced a number of outstanding condensed matter physicists, both theorists and experimentalists. In the last few years, with the ability of modern computational methods, especially based on density functional theory (DFT), theoretical work has had an increasing impact on our understanding of many of the more complex problems in condensed matter physics. One might be concerned, however, that this may lead to a disproportionate amount of theory work and thus an unhealthy numerical imbalance between theory and experiment. However, such an imbalance is not reflected in the individual programmes that were reviewed by the Panel; of these, about 1/3 belonged to theory, while the remainder were experiment-based. This seems to be an appropriate balance between theory and experiment and the ratio is similar to that found in other countries.

## Diversity of Research in Condensed Matter Physics

Sweden has a strong tradition of pioneering research in the areas of surface and materials physics and in spectroscopic techniques. As such, these areas form the major part of research in condensed matter physics. Theory and computation, particularly involving density functional theory, have always been strong in Sweden; and they continue to play an impressive role in shaping the interests of theorists and experimentalists alike. This is first-rate work, with strong scientific impact, which has been well funded in Sweden; so well, indeed, that there have been complaints of imbalance from those working in other areas of theory. While applauding the excellence of the DFT-related work, the Expert Panel also endorses the view that funding in one area should not be allowed to lead to weakening of otherwise strong activities in other excellent theoretical topics in theoretical condensed matter physics. Research in superconductivity (although diminishing in quantity), and in highly correlated electronic systems, is another area of activity. Magnetism, semiconductor physics, and the fashionable subfield of spintronics also flourish well in Sweden. Relatively speaking, soft-matter physics is not a dominant area of focus (at least as reflected by the Research Council grants evaluated), and neither is low temperature physics. Much of the recent effort, and the focus of many future plans, however, is in the popular area of nanoscience and nanotechnology. Swedish scientists are an integral part of the European thrust in nanoscience research, and participate in several collaborative research initiatives and consortia in the area. Nanoscience, like its predecessor surface science, is inherently multidisciplinary. Swedish physicists are certainly taking advantage of this cross-disciplinary nature of nanoscience, and have already ventured into the areas of biology, microelectronics, and engineering in close collaboration with experts in the respective fields. Because of the strength of achievements, and the leading role that Swedish scientists have played in surface science, they are in good position to play a leading role in shaping worldwide research in nanoscience and nanotechnology. On the applications side, several initiatives in this area are directed towards catalysis and energy related topics, but also topics in ecology, pharmacology, and medicine are emerging. The Swedish research community may gain from further focusing in these areas in the future.

## Size of the Groups

One concern raised by some researchers in condensed matter physics in Sweden was the relationship between the size of the groups and their ability to attract research funding. Some felt that funds are becoming

more concentrated on large groups or centres. Questions were raised as to whether a perceived policy of supporting strong and large groups at the expense of small ones was beneficial to the advancement of science or was instead pushing productive and talented researchers out of the research arena. While it is true that certain types of research activities benefit from collaborative efforts of a number of individuals, for other types creativity may flourish best under lone (or small group) efforts. Scientific survival should thus be made possible for both small and large units. In addition, in the case of large groups, it is important that there shall be a critical mass of individuals who bring in both coherence and diversity to the group, and that the group members have the possibility of achieving independence in the long run. The Expert Panel *recommends* that funding should be based on the quality of the proposed work, irrespective of whether the group is large or small.

### Long vs. Short Term Projects

A traditional virtue of the research environment in Europe has been the ability to pursue challenging, high-risk, high-gain, and long-term projects without the fear of losing funding mid-stream. This has worked to the benefit of science and society, as evident from several recent discoveries, e.g., high temperature superconductivity, scanning tunnelling microscopy, and giant magnetoresistance, all of which have had tremendous impact, and all of which matured in laboratories in Europe.

Sweden itself has been home to a remarkable number of innovations in condensed matter physics, both theoretical and experimental.

The present trend in Swedish universities is, however, a cause for concern. It appears that funding is generally for short term (two – three years) and is very competitive; and is mostly in the form of relatively low value grants. There is a general sense that far too much time is spent by scientists firstly in writing proposals to obtain research funds.

Because of the precarious employment conditions, which require university professors to acquire external funding for everything, including their salary, the short-term nature of the grants adds to their insecurity and impacts their working environment negatively. Since most students take four – five years to complete their doctoral research, the three-year duration of the grants is problematic.

These problems also impact on the choice of the projects undertaken by the researchers. Researchers are less willing to take on innovative but risky and very challenging projects for fear of losing their financial support (in case of slow productivity in the initial stages). If this trend continues,

Swedish scientists will have difficulty in continuing their efforts in fundamental and ground-breaking work, and the quality of research as a whole will suffer.

To address these problems, the Expert Panel *recommends* that funds should be made available for high-risk and long-term projects and that the duration of regular grants should be increased to four years.

## Interdisciplinary and Multi-Disciplinary Research

An important core of condensed matter physics research remains firmly implanted within the single discipline of physics, but increasingly it is at the boundaries with other disciplines that the important discoveries and applications are being made. This interdisciplinary character has been at the heart of surface science for some 40 years, and Swedish scientists have played a major role internationally in this area, both in developments of instrumentation and methods, and in exploiting these methods to gain insight into a range of phenomena relevant to physics, to chemistry, and to various aspects of materials engineering. The increasing emphasis on nanometre-scale phenomena and the associated technologies are increasing the need for interdisciplinary and multi-disciplinary studies, opening up new frontiers at the interface with the life sciences. The evidence from this review is that Swedish scientists have responded very positively to this challenge; and important new collaborations are making important inroads into these topics.

## International Visibility

There is no doubt that the Swedish condensed matter physics community does have significant international visibility. There are many indicators of this fact. In each area of expertise of the Expert Panel members, all from outside Sweden, the work of many of the Swedish groups was known to them, and indeed a significant subset of the relevant principal scientists were known to have presented invited papers at major international conferences. The publications of the groups are all in well-known and respected international journals. For the groups working in areas with clear potential applications, there is also a high level of participation in projects funded by the European Commission. Furthermore, applications for beam time at the ESRF by Nordsync scientists, a very significant fraction of which are from the Swedish condensed matter physics community, have a success rate high

enough to be awarded amounts of beam time significantly in excess of the time allocated to this network!

A further manifestation of the visibility of Swedish condensed matter physics is the very large number of applications to use the MAX-lab facilities for experiments in condensed matter physics by scientists from outside Sweden, not only from Europe, but also from the USA and Japan. In large part, this stems not only from the excellent facilities of MAX-lab, but also from the way that Swedish scientists have demonstrated the capability of this facility to perform experiments not readily performed elsewhere. In the light of these comments, one superficially surprising observation is that the number of articles by Swedish scientists in the CMP community in the most cited review journals (Physics Reports, Reports on Progress in Physics, and Reviews of Modern Physics) is low (less than ten during the last ten years), considering the otherwise high publication rate in prestigious journals, such as Physical Review Letters, Science, and Nature, by the community. One reason for this, which is known to have influenced some invited authors of such articles in Sweden, is the time needed to write a review paper, balanced against the perceived pressure to publish original science articles, and to write research grant proposals to ensure the salary of the scientist is properly funded. This seems to be yet another manifestation of the problems identified in the section on the “Employment structure...” as it operates in Sweden.

## Mobility and Interactions Within Sweden

In the written reports from the research groups, answers to the question “Describe, in order of priority, what you consider to be the weakness of Swedish Condensed Matter Physics” (see appendix 3) were included. In response to this question, quite a significant number of respondents raised criticisms; several grant holders have suggested that “a weakness of Swedish condensed matter physics is the lack of a national meeting within the community”. The written comments offer no clear explanation for this situation, and the issue was not discussed during the site visits because of the limited time. One researcher notes: “for some reason it has been impossible to get sufficient interest to establish a regular national meeting”. The Swedish Physical Society has ten different sections, of which Condensed Matter Physics is one. Several of the other sections, e.g., the sections for Atomic and Molecular Physics, and for Particle and Astroparticle Physics, have national meetings on a regular basis. In the US, the March meetings

sample condensed matter physics not only from the Division of Condensed Matter Physics of APS, but also from condensed matter physics in several other divisions.

It is not clear to the Expert Panel why there is a lack of interest in a national meeting in Sweden, but the Panel feels that such meeting could serve several purposes. It would possibly serve to increase the interaction between different Swedish groups, and it would make it possible for the community to act in a more concerted way.

The low mobility of staff in the Swedish research system is often highlighted in international evaluations; condensed matter physics is no exception. The new research career structure, implemented in 1999, which allows lecturers to be promoted to professors, and the slow but visible trend to make promoted professors equal to recruited professors, is commendable, but one obvious consequence is that it has decreased the already low mobility in Sweden. The problem is closely linked to the problems discussed in the section on "Employment structure". The problems must be solved in the correct order, and as long as the employment structure remains the main problem, the low mobility will remain an immediate consequence. There are physics departments where many faculty members have been recruited through the soft money entry during the last decade, with few positions announced for free competition. Such system does not promote mobility. Another trend seems to be that when a holder of one of the old type of professorships retires, the faculty funding is not used to recruit a new professor in full competition, but rather to cover the salaries of promoted professors. With almost no openings, the survival strategy of young researchers is to remain in their home universities where they received their Ph.D. Degrees.

## Infrastructure for Swedish Condensed Matter Physics Research

While the key component of research is skilled manpower, major items of equipment are essential for the pursuit of research in condensed matter physics, not only in experimental studies, but also in much of theoretical physics, which is dependent on large-scale computing. These are provided in Sweden, as elsewhere, through local equipment (located in the researcher's home university laboratories) and through shared national facilities. One feature of the means of local equipment provision in Sweden is that Swedish scientists heavily rely on the private Knut & Alice Wallenberg

Foundation for this support. So far, this system seems to work quite well in practice, although there is a continuous demand for further expenditure of this kind. More serious, curiously enough, is the funding of “medium-expensive” equipment (costing up to the lower limit for the Research Council expensive equipment of 2 MSEK). In principle, applications can be made to the Research Council for medium-expensive equipment, but in practice applications for manpower funding are typically favoured, particularly because most requests for manpower funding are to cover the salaries of existing University staff (see section: “employment structure”). The Expert Panel suggests that the Research Council should allocate additional funding for scientific equipment, in particular medium-expensive equipment. Such funding is, amongst other things, important for instrumental development projects, which otherwise can be difficult to fund. In Sweden, there are four main types of national infrastructure support, namely computing-, synchrotron radiation-, neutron- and clean rooms with micro- and nano-fabrication facilities. The main features of these are described below.

### National Computing Facilities

Sweden appears to have a very satisfactory range of different facilities for large-scale computing through SNIC, with a selection of high-performance computers in the form of various clusters. Computational physics plays a significant role in Swedish condensed matter physics, so such resources are important. The overall impression formed by discussions with the Expert Panel at all institutions visited was that computing resources were in no case limiting productivity. Of course, in many institutions these national facilities are complemented by local workstations and small computer clusters (and in one or two cases individual groups felt a lack of funds for more local clusters), yet overall it appears that the balance between local and national facilities, and the overall level of such resources, is about right.

### Synchrotron Radiation Facilities

Synchrotron radiation plays a major role in much of condensed matter physics, and particularly in the area of surface and interface science and electronic structure. The European Synchrotron Radiation Facility in Grenoble provides a third-generation source designed particularly for “hard” X-rays (especially for photon energies significantly greater than 10 keV), and Swedish scientists have access to this facility as members of the Nordsync consortium. In addition, however, in common with many European countries which also have national facilities (UK, France, Germany, Switzerland, Italy, Denmark,

soon to be joined by Spain), Sweden has MAX-lab, at Lund University, which has been an exceptionally successful and competitive facility. MAX-lab was first established with a low energy (550 MeV) essentially second-generation storage ring (predominantly using bending magnets as the radiation sources), with most beamlines devoted to photon energies below 100 – 200 eV for spectroscopy. During the early 1990s, MAX II, a 1.5 GeV third-generation source with undulators and multi-pole wigglers, was commissioned alongside the original MAX I ring, greatly enhancing the performance in the soft X-ray range in particular. This has been, and continues to be, an extremely successful and highly competitive facility, attracting large number of users from outside Sweden, and indeed outside Scandinavia. Especially through creative engineering, this facility has been built up, and operates, for a small fraction of the cost of facilities delivering similar performance elsewhere. In the recent (2002) review of Swedish National Laboratories, it was rated very highly and was indeed recommended to receive the largest increase of funding to enhance the very low levels of dedicated manpower for a user facility. MAX-lab is already in the process of constructing a new low emittance 700 MeV storage ring, MAX III. This new facility will give much-improved performance for low photon energies (below ~100 – 150 eV), of especial relevance to electronic “band mapping” in solids and surfaces, and is now developing the case for MAX IV; based on a novel double-ring design, which would serve both soft and hard X-ray users.

There is no doubt that the existence of MAX-lab and its synchrotron radiation sources has shaped a significant fraction of high-quality condensed matter physics research in Sweden, especially in the areas of surface and interface science and the electronic structure of solids. The strong tradition of spectroscopy in Sweden, combined with the availability of this state-of-the-art facility with beamline facilities, developed by both MAX-lab scientists and the user community, has placed several such groups in a world-leading position.

## Neutron Facilities

The Swedish condensed matter physics community has also had access to a national source of neutrons through the 50 MW reactor at the Studsvik Neutron Research Laboratory (NFL). The NFL is part of Uppsala University, although for all practical purposes as a user it is indistinguishable from a national laboratory. A primary mission of the NFL is to provide facilities for the Swedish community for neutron beam research. Fifty percent of the users are from Uppsala, thirty percent from other Swedish Universities, and twenty percent from the EU. The facility supports a broad range of spectro-

meters with wide-ranging capabilities, although the flux is deemed to be too low to support inelastic scattering studies. The recently appointed director of this facility, Adrian Rennie, is developing an increasing programme in investigations of soft condensed matter at the NFL. A secondary role of the NFL is to facilitate neutron-related research with the international community. Swedish scientists, for example, have collaborations with scientists at other international facilities, notably the ISIS spallation source at the Rutherford Appleton Laboratory, in the UK, and the reactor at ILL, at Grenoble in France. Unfortunately, during the course of this review, Studsvik AB, which operates the NFL reactor, announced that they plan to close this source during 2005. Thereafter, it would appear that all Swedish neutron scattering experiments in the future would have to use external sources unless, of course, Swedish aspirations to locate the proposed European Spallation Source (ESS) in Sweden bear fruit.

## Clean Rooms and Micro- and Nanofabrication Facilities

Much research in nanoscience and nanotechnology, and more specifically in semiconductor physics, and almost all research in semiconductor devices, heavily relies on access to clean room facilities and the microfabrication equipment installed in them. The very high capital and running costs of such facilities clearly means that they cannot be available in all institutions that need access to them, but the solution, which has evolved in Sweden, appears to be working well. In particular, there are three main centres possessing these specialised resources: the Semiconductor Laboratory at KTH in Stockholm, the Ångström Laboratory in Uppsala, and the Microtechnology Center at CTH (MC<sub>2</sub>) in Göteborg. A review of these three facilities was conducted by the Research Council in 2002, which made clear recommendations for them to be partly funded with a Swedish Nanotechnology Network (SNN) at an (minimum) annual level of 20 MSEK, and this has been implemented by the Research Council in association with other agencies. The specific purpose of the SNN is to provide facilities for qualified Swedish users from outside the host institutions and to avoid unnecessary duplication of effort. Within the SNN, the three facilities have complementary functions: the Semiconductor Laboratory at KTH is focused on microelectronics and photonics with strong connections with industry. The Ångström Laboratory is more concerned with multi-disciplinary R&D and associated education, exploring new applications in nanotechnology, biotechnology, and life science, and MC<sub>2</sub> focuses on the areas of high-speed electronics and nanoscale lithography. In addition, some local nanoscale fabrication facilities, which do not require expensive clean rooms, exist as

in-house facilities of varying scale in some of the other institutions, notably by Lars Samuelson at Lund University and David Haviland at KTH (Alba Nova), while the Department of Physics and Measurement Technology, Biology, and Chemistry (IFM) at LiU also has local clean room facilities for microfabrication. Overall, these facilities appear to more than fully satisfy the needs of the Swedish research community in this field. However, the Expert Panel foresees difficulties if the necessary funding for the maintenance and running of the large and expensive clean room facilities is lacking.

## Selection Procedure in the Swedish Research Council and Balance of Funding

It is not within the remit of the Expert Panel to assess the procedure by which projects in condensed matter physics are funded. However, in the section of the written reports submitted by grant holders, labelled “Scientific Part/Questions to each single grant holder”, one question was “Describe, in order of priority, what you consider to be the weakness of Swedish Condensed Matter Physics”. In response to this question, quite a significant number of respondents raised criticisms of the current assessment procedure, sometimes in a very outspoken manner.

The Expert Panel was confronted with further negative comments during the site visits. Although this issue is clearly outside the Panel’s terms of reference (the Panel lacks the detailed insight needed for a reliable assessment), it was felt inappropriate to ignore completely these rather severe criticisms. This short section therefore provides some comments and recommendations on this issue. It is not the intention of the Panel to respond to all comments provided by the researchers.

As there have been some changes in procedure in the recent past (some of which may address issues raised by the researchers), a few words on the current procedure of funding research projects in condensed matter physics are warranted, in order to put this matter in context. The research groups involved in the present evaluation receive their funding from essentially four review panels of the Scientific Council for Natural and Engineering Sciences (NT) within the Swedish Research Council. These panels are condensed matter physics (Bg O), materials science (Bg Q), engineering physics (Bg P), and semiconductor physics (Bg L). A few researchers funded from chemistry review panels were also included. Several groups are also funded by money from the Energy Committee of NT. The review panels

distribute funds to research projects in closed meetings, usually stretching over two days, based on written reports from the panel members and external reviewers. The chairperson of each panel is appointed by NT for a period of three years. The panel members are appointed for one year at a time by NT, based on the suggestions by an NT-council member within the area and by the chairperson. A person having an application being handled in a particular review panel cannot serve on the panel in that particular year; this also applies to the chairperson. During the review panel meeting, panel members having collaborations with applicants, or belonging to the same department as an applicant, must leave the room while the particular application is discussed. This is recorded for each application. For each application, the review panel must reach a consensus on what written report best reflects the opinion of the panel. This written report may be modified if needed. It is this single, written report, which the applicant is given and from which he/she has to decipher why the application was rejected or rewarded. The Research Council-system does not have project officers that can guide or advise the applicant, should his/her application be rejected or funded at a lower level. There are no detailed minutes produced during a review panel meeting.

Initially, we are addressing some technical issues, expressed in the comments from grant holders:

- It has been commented that the quality of the evaluations are lower now as compared with the situation in the past. The Expert Panel is not in a position to comment on whether this is, or is not, correct; however, it appears that the written reports by the review panel members were longer and more detailed in the past. This made it easier for a person to understand why an application was rejected or not funded at the desired level.
- Minutes cannot be used to check that the system is fair, as suggested by one commentator, since there are no minutes produced. However, the Expert Panel does not suggest that minutes should be produced. It would entail considerable additional work and would probably inhibit the free discussion needed to reach a consensus decision.
- The past record of an applicant is part of the criteria used by the review panel. The Expert Panel feels that an evaluation after a project has been completed, as was proposed by a grant holder, is redundant.
- One commentator suggested that, because funding to condensed matter physics is channelled through several review panels, the system may not be well suited for interdisciplinary research. The Expert Panel agrees that this is a relevant concern and advises NT to look into this issue.
- A more problematic point is the one of multiple contracts. The Research

Council currently has the policy that only exceptionally should there be more than one active contract per researcher. However, by making applications to several different review panels, astute researchers can currently “play the system” and accumulate as many as three or more contracts. This situation may also encourage researchers to spread their efforts more thinly – not necessarily very desirable – although, of course, some interdisciplinary research may naturally fall into the areas of several different review panels. The Expert Panel *recommends* that the Scientific Council for Natural and Engineering Sciences (NT) carefully review this policy. A strict one contract per researcher policy is certainly unambiguous and easy to control, and apparently adopted in the chemistry review panels; on the other hand, there could be arguments for multiple grants, such as the facilitating movement or collaborations between different research areas.

Several comments contained serious structural criticisms. If one were to take these comments at face value, a picture emerges of a system in which a small group of people has controlled the review panels for a long time, something that has resulted in all sorts of detrimental effects for condensed matter physics in Sweden. The Expert Panel is not in a position to assess whether these rather harsh statements are correct, or contain a core of truth. Some of the detrimental effects suggested in the comments are such that the Panel cannot agree with them. There is certainly a correlation between funding level and international ranking; the Panel did not find funding locked up in research, which is not of excellent quality. It would be too simple to say there is “no smoke without fire”. In general, it is obvious that a person who has served on a review panel better understands how a review panel works, has been confronted by a large number of applications of different quality, and knows from this experience how a good application should be written. Having made this obvious observation, the Expert Panel would *recommend* the following:

- i. The NT-council should consider increasing the international participation in some review panels. Perhaps increasing the presence of members of the other Scandinavian countries would be an interesting and practical possibility.
- ii. The review panel chairpersons should be instructed to consider carefully the geographic coverage when proposing the domestic membership of the review panel.

Finally, some comments seem appropriate on the problems associated with a situation in which the success rate drops below 10%. The Expert Panel agrees that it becomes increasingly difficult to select the best proposals, and there is a clear risk that the selection may appear random. The Panel also agrees that a programme with a 3% success rate, involving applications from hundreds of research groups and a massive amount of evaluation work, does seem like a poor investment in time and money.

# TOPIC AREAS

As discussed in the introduction, the Condensed Matter Physics area is very wide. In the following sections, we have divided the whole area into seven subareas:

- Surface Science, Interface Science , and Thin Films
- Nanoscience and Nanotechnology
- Magnetism and Spintronics
- Semiconductors
- Superconductors
- Condensed Matter Theory
- Soft Matter and Biophysics.

In the sections below, each subarea is firstly described historically and from an international perspective, followed by a description of the activities in Sweden within this subarea. In these descriptions, we also try to highlight what the Panel judged to be high-quality activities. Finally, under each subarea is a section named “future perspectives”, in which we discuss some of the present challenges within the area and, in some cases, also some recommendations regarding funding.

Since the evaluated entities have been groups or divisions rather than single grant holders, it is not as straightforward to use the same assessments as in the “standard type” of evaluations performed so far by the Research Council (see for instance the evaluation of Biotechnology), in which single grant holders are evaluated, according to a pre-set scheme. In the present evaluation, all the groups are mentioned somewhere below, mostly with some judgmental statement or recommendation. However, the focus of this evaluation has been on the research performed within the area, the prerequisites for the researcher to perform, and the Swedish Research Council’s role in all of this. The focus has not been to compare individual researchers as is, in principle, done every year in the review panels for the applications. In some cases, individual researchers within the groups are mentioned, but this is not exhaustive, and there was no intention to go systematically into each grant holder’s activity. In many cases below, where the Panel felt it appropriate, the judgmental terms used are those of the Research Council-standard evaluations, namely, “outstanding”, “excellent”, etc., but other terms are also used. The general objective was to perform as balanced a view of the research area as possible. The judgmental terms

“internationally leading” and “internationally competitive” correspond roughly to the Research Council-defined terms “outstanding” and “excellent”, respectively, but sometimes the discussion is of groups, and sometimes of projects or individual researchers. Groups or individuals may be mentioned in more than one section below, since their activities are not always limited to one of these subareas, and judgmental statements may vary correspondingly, reflecting the evaluation of the contributions to the different subareas.

## Surface Science, Interface Science and Thin Films

### International Perspective

The “birth” of modern surface science can be defined by the development of commercial demountable and bakeable stainless steel ultra-high vacuum (UHV) chambers and ion pumps in the 1960s, making possible, in a relatively routine fashion, the application of far more complex experimental methods than had been possible in glass. There followed an extended period of 10–20 years, in which a whole range of specialised, surface-specific techniques was developed. Initially, low energy electron diffraction and the electron spectroscopies of photoemission and Auger electron emission blossoming into a range of electronic and vibrational spectroscopies, a number of quantitative structural techniques based on conventional diffraction of electrons, X-rays and atoms, and on local scattering of electrons and ions, as well as molecular beam methods for investigating surface chemistry. In the 1980's and 1990's, synchrotron radiation played an increasingly important role in some of these areas, stemming from the high spectral brilliance, very wide-range tunability (far IR to hard X-rays) and potential for high spectral resolution of this source of radiation. The 1990's saw a huge expansion in the use of scanning probe microscopies, and especially scanning tunnelling microscopy (STM), invented by Rohrer and Binnig a decade earlier (for which they received the Nobel Prize in Physics, in 1986). There is no doubt that STM has had a pivotal role in advancing our understanding of a range of surface phenomena, and its use now pervades much of the research in this field, yet the great majority of such work remains qualitative in character, and the results of spectroscopic and true structure determinations, as well as of surface kinetics and dynamics, still form the quantitative base of the subject and the strongest links with theory.

The last decade or so of surface and interface science has been marked by two particular trends. One is to problems of increasing complexity. A major driving force for much of surface science has been the desire to gain a fundamental understanding of heterogeneous catalysis, and much work has been directed to this aim. In the early years, though, surface science focused on the very simplest model systems – not only low index single crystal surfaces in UHV, but also only simple atomic and molecular adsorption. With the confidence gained in this underpinning work, and the benefit of a wider range of complementary, and more incisive, techniques, problems of greater complexity, such as coadsorption phases, or even surfaces under reaction conditions, are increasingly addressed. Other examples of more complex surfaces include work on films of relatively complex organic molecules, such as those with potential for molecular electronics, or, indeed, increasing amounts of work on the surfaces of epitaxial films, especially of oxides. The second trend concerns the interface between surface science and nanoscience. Nanoscience is concerned with systems of much reduced size in one, two, or three dimensions, and surfaces are intrinsically systems with a small dimension in one direction. Many of the experimental methods of nanoscience derive from surface science, and one area of increased complexity in surfaces is the study of surface features with reduced lateral dimensions – nanowires and nanoclusters. The increased use of scanning probe microscopies with lateral resolution of atomic dimensions provides the strongest cross-link between the two fields. As such, while nanoscience and surface science are certainly not equivalent, there is a significant subfield, which could equally well be described by either of these names. In this section, we concentrate on those aspects of surface science not generally classified as nanoscience. A separate section is devoted to nanoscale phenomena.

One further important development in the field of surface science is the growing impact of density functional theory. The combination of advances in DFT and the ready availability of fast computing facilities has meant that it is now possible to calculate not only equilibrium (minimum energy) surface structures, including those of transition metals, but also detailed aspects of surface dynamics, reaction transition states, etc. Not only are important advances being achieved through experiment – theory collaborations, but also, in some cases, this kind of theory is being integrated into experimental groups.

Within this topical overview has also been included some work in the area of thin films. This is a very broad area in general, which includes not only aspects of surface science, but also much materials science embracing electronic and functional materials. Some aspects of thin film work specifically exploit the coating nature of these films for chemical or mechanical

protection, and for optical properties, whereas in other cases one is primarily interested in the bulk properties of the material, yet the growth of the material (often in metastable phases) exploits thin film deposition methods. Much work in this field falls naturally into the topics of semiconductors, magnetism, and nanostructures, which are dealt with elsewhere; those topics, less easily classified in this way, are further discussed below.

## Surface Science, Interface Science and Thin Films in Sweden

Surface science remains strong in Sweden; indeed, this is certainly one of the strongest areas of condensed matter physics in Sweden. In part, this stems from the traditional strength in electron spectroscopy, and there is no doubt that some Swedish groups continue to play a leading role on the world stage in developing new and existing electron and related spectroscopies. In the 1992 review of Swedish research in physics, the Expert Panel questioned whether this work did not play an unreasonably dominant role in Swedish condensed matter physics research. In the meantime, a number of important changes have taken place. Firstly, there have been major developments at MAX-lab, including the building and commissioning of MAX II and related beamlines. This has created such a favourable environment for photoemission, X-ray absorption, and the newly exploited X-ray emission spectroscopies that it would be unreasonable if Swedish scientists did not exploit this remarkable advantage; many groups from outside the Nordic countries have come to MAX-lab to follow the lead of Swedish groups in exploiting the methods developed. On the other hand, while most Swedish surface scientists do make use of these techniques, they have also broadened their base in terms of methods and applications, and the majority of such work is now clearly directed to solving problems with the methods rather than primarily focusing on the spectroscopies *per se*. For example, notable relative to the comments of the 1992 report is the widespread, but balanced, use of STM. There is also a significant component of the work in these spectroscopies being directed to an understanding of bulk electronic structure, a trend that may be seen elsewhere, particularly since the discovery of high-temperature ceramic superconductors.

Much of Swedish surface science also reflects the international trend to investigate systems of greater complexity, and indeed, in some cases, to apply methods developed in the context of surface science to study sub-surface phenomena. Examples include some relatively complex molecular adsorbates, including work on quite fundamental physics applied to complex systems, such as dye molecules on solar cell materials, studies of surface dynamics, and work directed to understanding surface phenomena at much

higher pressures than traditional UHV studies. Swedish surface science also reflects the increasing role of theory – experiment collaboration and integration; there is a long history of a major role of theory in this area in Sweden, and this continues to flourish. The work in this general area can usefully be subdivided into six themes, namely instrumentation and methods, electronic structure, surface chemistry and dynamics, geometrical structure, applied surface science, and theory. Theory interacts strongly with experiments, thus it could be included within the other themes – yet some comments on the overall state of Swedish surface science theory appear appropriate. Finally, some work on thin films is discussed.

### Instrumentation and Methods

In many ways, the pioneering work in Sweden on the development of instrumentation and methods relevant to surface and interface science follows the long tradition of developments in electron spectroscopy in this country. The achievements are no less for this – their positive impact can now be seen in work performed by many groups worldwide, which have assimilated these developments. A particularly obvious example is that of the very widespread use of the Scienta hemispherical electron energy analysers in surface electron spectroscopy, especially at synchrotron radiation facilities; these instruments derive directly from the developmental work conducted by the Surface Physics group at Uppsala University (headed by Nils Mårtensson), which has an outstanding impact. A second such example is the development of both the technique and the associated instrumentation for X-ray emission spectroscopy (XES) and the related method of resonant inelastic X-ray scattering (RIXS) by the Soft X-ray Physics group at Uppsala University (Joseph Nordgren). This technique provides unique information on the localised valence electron structure in solids. Despite the very low cross-section for XES in the soft X-ray energy range, this technique has been shown by this group to be so successful that it is being adopted by many groups outside Sweden; here too, the international impact has been outstanding. Indeed, through work in these groups at Uppsala University, involving Anders Nilsson (now at Stockholm University and Stanford University), it has even been found possible to apply these methods to investigate submonolayer coverages of molecular adsorbates and provide new insight into the bonding mechanisms. The Electron Spectroscopy and Molecular Surface Physics group at Uppsala University (Hans Siegbahn) has also played a leading role in the application of electron spectroscopy to liquid surfaces.

The very important role that the MAX-lab facilities have had in helping Swedish scientists to play such an important role in the application of synchrotron radiation to surface science, also owes much to the work

performed by Swedish university groups in developing beamlines and associated end-stations. Important contributions of this kind have come from the Materials Physics group at KTH (Ulf Karlsson), the Synchrotron Radiation research group at Lund University (Jesper Andersen), the Electronic Structure of Condensed Matter (Per-Olof Nilsson) and Solid State Physics (Lars Walldén) groups at CTH, the Surface and Semiconductor group (Roger Uhrberg), the Materials Science Division (Leif Johansson) and the Thin Film Physics Division (Jens Birch) at Linköping University, as well as the major effort from the Uppsala University groups. The effective implementation of specific beamline designs at MAX-lab has done much to bring about world-leading applications of existing techniques as well as new methods. For example, the Surface Physics group at Uppsala University made pioneering demonstrations of the ability to use shifts in core level photoelectron binding energies to distinguish between different adsorption sites of the same species on surfaces (through both adsorbate and substrate photoemission signals) using a laboratory-based rotating anode XPS instrument. It was then the high-resolution soft X-ray beamline BL22 on MAX I, used especially by the Lund University group and co-workers, which demonstrated the full power of this method for unravelling quite complex surface chemical reactions and providing important qualitative surface structural information, a method now used with even greater effect on MAX II beamlines. This approach is now increasingly used at other facilities.

Another spectroscopy which has been skilfully developed in Sweden, is high-resolution electron energy loss spectroscopy, within the Surface Physics group of Stig Andersson at CTH, which currently possesses one of the best HREELS instruments in the world. Through this instrumental development, research topics of a quite fundamental character have been addressed, including coherent quantum scattering at surfaces involving heavier atoms and small molecules.

During the early development of scanning probe microscopies, Sweden had a group on atomic force microscopy instrumentation led by Ragnar Erlandsson (Linköping University), which at the time contributed strongly to developments in the field. This research effort is now terminated. A related activity is the combined TEM/STM instrumentation developed at CTH by Håkan Olin, Krister Svensson, and Eva Olsson. This excellent development has resulted in new and outstanding scientific applications including the nanopipette deposition/removal of metals at surfaces.

### Electronic Structure

The historical strength of Swedish electron spectroscopy is perhaps most obviously manifested in the work on the electronic structure of surfaces

and of solids by surface methods. In the case of core level spectroscopies (including XPS, X-ray absorption spectroscopy (XAFS), XES, and RIXS), the Uppsala groups have been particularly effective in exploiting their pioneering efforts in the development of the associated instrumentation and methods. Of especial note here is the development of the “core-hole clock” technique by the Mårtensson group to study electron dynamics, and also put to good use by the Siegbahn group and Mats Fahlman *et al.* As remarked above, the development of XES and RIXS by the Nordgren group has had a major impact on the ability to obtain valence electronic structure information in an element-specific local fashion. Anders Nilsson, now at Stockholm University and Stanford University, but originally in the Mårtensson group at Uppsala University, has been especially effective in gaining an improved understanding of molecular bonding at surfaces using a combination of these experimental methods and DFT calculations, and their excellent work on molecular bonding in water is already being heavily cited, a clear indication of its outstanding international impact.

More direct probing of the valence electronic structure using ultra-violet photoemission has also been pursued with great success by several Swedish groups. W.R. Salaneck at Linköping University has been particularly effective in applying this method to the study of conducting polymers over many years, using novel methods for *in situ* deposition of the films, and he has a world-leading position in this field. The groups of Per-Olof Nilsson and Lars Walldén at CTH have a very long record of achievement in the application of photoemission to study electronic structure. Walldén’s recent excellent work on quantum well photoemission in alkali metal films exemplifies the depth of understanding that can be achieved by studying well-chosen model systems with great care and in detail. Janusz Kanski in the Per-Olof Nilsson group has been extremely successful in developing an almost unique capability for *in situ* MBE growth of semiconductors on MAX beamlines to investigate Si delta-layers in GaAs, and recently to grow GaMnAs material of unsurpassed quality. Other examples of very good studies of semiconductor surface electronic structure by photoemission include the work on Si and Ge surfaces by Roger Uhrberg at Linköping University (LiU); on SiC surfaces and interfaces, by Leif Johansson (LiU); on alkali metals on Si and on SiC surfaces by Lars Johansson at Karlstad University; and on Ge/Sn surfaces by the KTH group of Ulf Karlsson; this group has also had notable success in the use of pump-probe two-photon photoemission to study the dynamics of excited states in these systems. A further particularly interesting and excellent recent development by this group (Oscar Tjernberg) is the use of relatively high-energy valence band photoemission in combination with a 2D detector in a hemispherical

electron energy analysis to achieve “one-shot” band mapping of several model surfaces; this could prove an extremely interesting development for the future. A quite different topic of study in electronic structure from within the CTH group of Per-Olof Nilsson is the very good work on alkali-intercalated layer compounds by Hans Starnberg; a particularly interesting recent aspect of this work is the use of photoelectron microscopy at MAX-lab to gain further information of the mechanisms involved in the intercalation process. Finally, within this context we should note the work going on within the Nils Mårtensson group (Uppsala University) on magnetic properties, in part through the very good programme of work on magnetic dichroism using the new variable-polarisation beamline set up by this group at MAX II, but also the exploratory work to investigate coherent magnetic speckle in collaboration with Kevan’s group, working at the ALS. This latter development is in an early stage, but has the potential to have an outstanding impact.

### Surface Chemistry & Dynamics

One of the driving forces for the growth of surface science was the potential to understand surface chemical reactions and fundamental processes in heterogeneous catalysis. While appropriately labelled surface chemistry, this topic lies at the heart of much interdisciplinary surface science, and as such is generally regarded as an integral part of condensed matter physics. Here too, electron spectroscopy using synchrotron radiation plays an important role, although there is also a very significant body of home-laboratory-based experimentation of very high quality. Groups contributing very good work to this area include those of Nils Mårtensson at Uppsala University (UU), Ulf Karlsson (KTH), and Hans Siegbahn (UU) – in this case work on CVD precursor surface chemistry – and that of Jesper Andersen at Lund University (LU), which has made outstanding contributions in exploiting adsorbate and surface photoelectron core level shifts, as mentioned earlier. This latter group has also recently been performing X-ray diffraction studies at elevated pressures to address the “pressure gap” in heterogeneous catalysis, specifically in the context of surface oxide formation, using the ESRF (Grenoble) and ANKA (Germany) synchrotron radiation facilities. This is an excellent contribution to a field of growing importance.

Of course, the traditional methods for studying heterogeneous catalysis are concerned more with the chemical kinetics, and the group of Bengt Kasemo at CTH has been very successful in an excellent programme which combines such experimental studies of novel model systems with theoretical modelling to gain greater insight into associated mechanisms. This group has also made significant impact through molecular beam

scattering studies on model single crystal surfaces, using more conventional surface science methods and particularly through collaboration with the theory group of Bengt Lundqvist at CTH, to gain further insight into surface chemical dynamics. Understanding surface molecular dynamics also lies at the heart of the work of Stig Andersson at CTH, studying the fine details of hydrogen on surfaces using high-resolution electron energy loss spectroscopy at ultra-low temperatures; these are excellent and very elegant experiments in a field where such information is much needed. A quite different kind of simple model system with which to tackle the fundamentals of heterogeneous catalysis is through the use of naked metal clusters, initially in the gas phase, but also deposited in a controlled fashion on surfaces. The Molecular Physics group at CTH (Arne Rosén) has had some notable successes in some excellent work exploiting this approach (and comparative studies of extended surfaces). It is also notable that the UU group of Nils Mårtensson has initiated a programme of studies of clusters relatively recently.

A strong surface chemistry activity in Sweden has been the polymer–metal interface research effort by W.R. Salaneck and co-workers at LiU in collaboration with Mats Fahlman *et al.*, currently at Campus Norrköping. The activity has through its experimental work – mainly based on photoelectron spectroscopy and collaboration with theoretical groups abroad – strongly contributed to the understanding of the properties of these interfaces. Important aspects have been nature of added-electrons in conjugated molecules and polymers, band alignment and ultra-fast charge transfer at polymer–metal interfaces. This research activity is also an example of the interplay between basic surface science and applied surface science. The group has had strong collaborations with the EU and with industrial partners in the fields of molecular electronics and solar cell applications, and their overall impact in this field has been outstanding. Promising work on polymer systems for electronic properties is also being initiated in the group at Karlstad University (Ellen Moons).

A quite different spectroscopic approach to the study of surface chemistry is through the use of infrared absorption–reflection spectroscopy. The very high spectral resolution achievable by this method offers significant advantages for the study of complex systems. In the past, however, the understanding of the intensity of fundamental, combination, and overtone bands has placed significant limitations on the quantitative use of this method. The excellent work of Per Uvdal (LU) in gaining a proper theoretical description of these effects in a number of model systems studied, using instrumentation of unparalleled performance, is of great importance in this regard.

Work on heterogeneous catalysis is also being pursued by the Surface Chemistry group (Anders Palmqvist) at CTH, but the only Research Council-funded work in this group is concerned with chemical synthesis, which falls in an area outside the range of competence of the Expert Panel.

### Geometrical Structure

The atomic positions of atoms in a surface are a starting point for a theoretical understanding of many other properties of the surface, including the electronic structure and the chemical activity. In the early days of the development of quantitative LEED methods, there were several groups active in Sweden in this field. Currently, the only quantitative surface structure work being pursued by Swedish groups appears to be the application of surface X-ray diffraction of surface oxidation by the Lund University group of Jesper Andersen, mentioned above (a group also with past experience in quantitative LEED studies). Nevertheless, there are quite a number of activities in Sweden related to qualitative or semi-quantitative methods to elucidate aspects of surface structure. The use of surface and chemical shifts in photoelectron binding energies by Andersen's group at LU, and others, mentioned above, is a case of ongoing pioneering work to gain adsorption site information in a less direct but simpler fashion. There is also a substantial body of somewhat similar, very good work by Roger Uhrberg (LiU), in using detailed investigations on surface core level shifts to elucidate the structure of Si and Ge surfaces, and by Leif Johansson (LiU) studying Be and SiC surfaces. While STM can also provide surface structural information, there is great scope to misinterpret such atomic-scale images and the collaboration between Mats Göthelid (KTH) and Susanne Mirbt (UU) to both measure and model STM images of the InAs(100) surface is an important development to address this problem. Several other groups are also using STM, as a valuable aid to understanding structure; the very good work using cross-sectional STM by the group of Jesper Andersen at LU, to investigate nanostructured materials produced by the Lars Samuelson group at LU is a particularly elegant and demanding application.

More quantitative structural information can also be extracted from selected spectroscopies. Polarisation angle dependence in near-edge XAFS can be used to gain valuable information on molecular orientations at surfaces and is the theme of a very good collaboration between the group of Lars Johansson (with Ellen Moons) at Karlstad University and Michael Grunze in Heidelberg, on alkane thiol self-assembled monolayers. This group also continues to explore the use of photoelectron diffraction, which can give complete quantitative structure determination.

## Applied Surface Science

Defining what is basic surface science and what is applied science is clearly somewhat subjective, but a common line is drawn between investigations of surfaces prepared and modified under UHV conditions (usually single crystal surfaces), and *ex situ* analysis using surface spectroscopies of more complex materials, commonly prepared in air, in solution, or in more hostile environments. This definition probable excludes most of the work supported by the Swedish Research Council in condensed matter physics. There are, however, some important exceptions. For example, the very good work of the Siegbahn group at UU on dye-sensitised solar cells and vascular stents falls into the category, although in the case of the dye work parallel studies on well-characterised surfaces – which are more overtly mainstream surface science – play an important role in the data interpretation. Both systems are interesting examples of modest but significant developments of existing methods of applied surface science to study complex “real” materials, and as such define a valuable trend.

Much of the work of W. Salaneck (LiU) and Mats Fahlman (Campus Norrköping), some of which is described in the previous section, is rooted in a range of applications. Here, too, they have applied the core-hole clock technique to investigate the dynamics of dye-sensitised solar cells, notably in hybrid devices, in which the liquid electrolyte of a conventional Grätzel cell is replaced by conducting polymers. Photoemission is also being used to study pi-conjugated organic molecules of interest for molecular electronics, as well in materials development for polymer light-emitting displays. Much of the finance for this excellent work comes from EC-funded projects, yet it is the Swedish Research Council-funding, which provides the underpinning science that puts the group in a position to bid for these additional external funds. As such, the funding from the Swedish Research Council provides considerable leverage.

A rather different example is contained in the work of the Nordgren (UU) group using XES and RIXS. The use of photon-in/photon-out methods mean that many of the usual constraints of ultra-high vacuum are no longer implicit in the application of the method, and exploring the use of these methods to more complex non-UHV situations is important. A particularly elegant and fruitful example of this, is their very good investigation of the way Fe can reduce higher oxides of uranium through the use of a cell containing the solution of the uranium salts with a thin Fe film coating the inside of the X-ray window; the results of potentially of great significance in the long-term storage of nuclear waste.

## Theory

An increasing trend in surface science is the use of theory – especially density functional theory – in parallel with experiments, to gain far greater insight into underlying physical mechanisms and processes. While there is a separate review of theory in general within this report, some comments on the impact of Swedish theory in surface and interface science appear appropriate here. Some relevant theory/experiment collaborations have already been highlighted above, such as those within individual groups (e.g., Anders Nilsson's group at SU), between groups in the same institution (e.g., the collaboration between the groups of Bengt Kasemo and Bengt Lundqvist at CTH on surface dynamics) and between groups in different institutions within Sweden (e.g., Mats Göthelid at KTH and Susanne Mirbt at UU on STM image interpretation). Other activities in these categories are the combination of theory (Bo Hellsing), and experiment addressing lifetime broadening in surface states and quantum well states in Wallden's group at CTH, and the investigations of energy shifts in photoemission core level spectra of clean and adsorbate covered surfaces at LU (Jesper Andersen and Carl-Olof Almbladh).

There are also examples of important theoretical work based on international collaborations, and others without such collaboration, which have nevertheless had significant general impact in surface science. Of especial note is the work of Mats Persson in the group of Lundqvist at CTH on single-molecule vibrational spectroscopy in STM, and related phenomena discovered in some of the experiments of Wilson Ho in the USA. These are hugely important experimental developments, now being exploited by several groups in Europe and Japan, which lacked the firm footing of theoretical understanding; this theory is thus of great general importance with an outstanding impact. The group of Börje Johansson (UU) has also made some excellent contributions in the area of surface science; this group first addressed the problem of understanding surface segregation and photoelectron binding energy chemical shifts in a semi-empirical fashion many years ago, but are now making valuable contributions to these topics through *ab initio* methods. Experimental groups (Jesper Andersen *et al.*, LU) are also working along these lines in collaboration with theoretical groups abroad (M. Scheffler, and G. Kresse).

A strong point in theoretical surface physics in Sweden is the outstanding research activity in the Lundqvist group at CTH, including the work by Mats Persson, mentioned above. The group addresses the leading fundamental issues in surface and materials science, which also find relevance in industrial application, e.g., the theoretical work on accurate determination of the structure of alumina. Other examples are: understanding the nature of

hydrogen bonding for water molecules, epitaxial growth on selected surfaces, quantum and classical behaviour of hydrogen dynamics on metal surfaces, and the water production reaction on Pt. Theoretical developments to include dispersion forces into DFT calculations by the group is of utmost importance in treating a range of molecular systems at surfaces.

### Thin Films

Within the field of thin films in Sweden, not covered by the Semiconductor Physics and Magnetism sections in this report, two groups are concerned with rather different aspects of the optical properties of such films. The group of Hans Arwin at Linköping University strongly focuses on applications of ellipsometry on surfaces and thin films. Ellipsometry in the infrared to near ultra-violet spectral range is well known to be remarkably sensitive to even submonolayer coverages of adsorbates on surfaces. This group has specialised in developing and applying this method to a wide range of problems, recently including organic and bio-material films, extending to film thicknesses of 100s of microns. This is good work exploring an increasing range of applications. At Uppsala University, the group led by Claes-Göran Granqvist is also concerned with optical properties of materials. One strong effort in the group is directed towards solar energy applications, another is “smart windows”, based on electrochromics. The group, doing mainly experimental work, covers a range of activities aimed at understanding basic properties of optical bandgap materials, optical modelling and coatings and materials for a range of applications. Recently, a new promising activity in pharmaceutical materials has been initiated. This is a group with very strong interactions with industry, leading to examples of excellent applied science. The group is another example where the Research Council-funding for understanding physical processes underpins their more applied work.

A quite different activity in the area of thin films is the group led by Lars Hultman at Linköping University. This is a group more overtly concerned with exploring and exploiting the methodology of thin film deposition to create new materials, including novel nitrides and ultra-hard coatings. The activity covers materials synthesis and characterisation as well as computation and modelling. This is important applied science, with clear roots in fundamental understanding of the underlying physics and exploitation of the varied deposition methods – and thus is making an excellent contribution to this field.

### Future Perspectives

It is always dangerous to try to predict the future. However, a few issues within the surface and interface field are reasonably clear. Firstly, with

MAX-lab continuing to develop (new stations for both MAX II and MAX III are being, or will be, implemented in the next one – three years), one can anticipate that the very successful surface science studies that exploit synchrotron radiation will continue to flourish. Several groups at Uppsala University (Mårtensson, Nordgren, Siegbahn), as well as the Lund synchrotron radiation group of Jesper Andersen, are further developing the ability to investigate surfaces at “high” pressures, of increasing relevance to “real” or practical surface applications. MAX IV, if funded, will enhance the ability to perform core level photoemission investigations of subsurface phenomena through the use of higher energies, allowing further applications into more complex phenomena.

A quite different issue, which will change the face of Swedish surface science, is that of staff retirements. As in many Western countries, there was a significant expansion of higher education in Sweden in the 1960's and 1970's, bringing with it an influx of new young academics. Coinciding, as it did, with the “birth” of modern surface science, a very significant number of these appointments fell in this research area. In the next five years or so, many of these academics, which have been leading scientists of the international research community, will retire. For example, at CTH this includes Bengt Lundqvist, Per-Olof Nilsson, Lars Walldén, and Stig Andersson. Several other examples can be found in other institutions. In some cases, there are already younger academics in place in these groups with a high research profile, who could naturally take over the important roles vacated; in other cases, there is no such natural progression. In many of these institutions, as described in the “General Recommendations” section, there is an excess of staff on nominally permanent positions that rely entirely or mainly on external funding for their salaries, but who may be in quite different research areas. There is a real danger, therefore, that some existing strengths of this area of Swedish condensed matter physics will be lost through default, rather than through conscious planning. It would be very regrettable if this were allowed to happen.

For future development of materials with novel physical properties, strong competence in thin film growth is a prerequisite. Sweden has such competence, which should be allowed to develop in the years to come.

As in all areas of condensed matter physics research, the overriding issue in funding is that of staff salaries. There is clearly a long-term problem here, which is in danger of having a growing negative impact on the ability to maintain the current level of research activity. Any reduction of funding would be highly regrettable. The overall quality of surface and interface science research in Sweden is very high, and there is certainly no individual activity, which could be regarded as of too low a quality to deserve adequate

funding. The strong connection of this community to the utilisation of MAX-lab is also a major factor in defining funding priorities. On the one hand, it is clear that such a valuable national resource should not be wasted by inadequate funding of the user community. On the other hand, it would be quite wrong to make Swedish surface science a monoculture that is *only* based on synchrotron radiation studies.

## Nanoscience and Nanotechnology

### International Perspective

The vision of nanoscience is often traced to a 1959 lecture by Richard Feynman entitled “There is a lot of room at the bottom: an invitation to do a new kind of physics,” in which he predicted that the day was not far away when one would be able to build material atom-by-atom. There is little doubt that without the blessings of Feynman, nanoscience would not have had such global acceptance and appeal, but in all fairness, the present interest in and euphoria about nanoscience and nanotechnology is also the outcome of several decades of gratifying experimental and theoretical advances in the areas of surfaces, interfaces, and atomic clusters. Since the early seventies, a series of developments in experimental techniques made possible the examination of phenomena at surfaces with sub-nanometre sensitivity. While earlier advances were mostly in spectroscopic techniques, the invention of the scanning tunnelling microscope (STM) in 1982, by Gerd Binnig and Heinrich Rohrer, made direct (real space) observations feasible and attractive. STM became a household word in 1990, with Don Eigler’s gallery of images created by moving atoms (Xe) and molecules (CO) on metal surfaces with the STM tip, turning Feynman’s prophecy into reality. Now, a whole plethora of techniques known collectively as scanning probe microscopy (SPM) are commercially available and have found applications way beyond the confines of surface physics. Another traditional area of relevance to nanoscience, cluster physics, also received a big boost with the discovery by Harold Kroto and Richard Smalley of the fascinating structures and novel properties of fullerenes, the  $C_{60}$  and  $C_{70}$  molecules. At the same time, at the applications level, K. Eric Drexler’s 1987 book “Engines of Creation”, brought forth some interesting and controversial ideas about nanotechnology. As science advisor to the US President, Bill Clinton, Neal Lane took advantage of these developments to convince Clinton and others that Nanoscience and Nanotechnology were the promise of the future. While worldwide efforts in nanoscience, particularly in Japan and several European countries, had begun some time

before, Clinton's signing of the nanoscience and nanotechnology initiative (NNI) in 2001 led to further impetus, as governments across the globe began to take keen interest in the subject and new funds for research in the area were made available. At this point, nanoscience and nanotechnology are not only a focal point for research worldwide, but they are fast becoming a part of the college (and in some cases high school) curriculum.

Over the last decade, the European Union has also established a strong knowledge-based research programme in nanoscience. National and regional policies and programmes have an important place in funding nanotechnology R&D. The EC contribution under FP6 amounts to about one third of the overall European expenditure in nanotechnology. The overall level of public expenditure in 2003 for Europe was 1100 M€ (EC 350 M€); Japan (810 M€); USA 1100 M€ (Federal 770 M€); and others 510 M€. In Sweden, the public funding in 2003 was about 15 M€ (Belgium 15 M€; and the Netherlands 50 M€).

What is nanoscience? Certainly, it has to do with properties at a length scale of 1 – 100 nm, but importantly, there is an expectation of novel properties of systems with at least one characteristic length on the nm scale. Thus very thin films, atomically corrugated surfaces, nano-sized atomic clusters, assemblies of molecular materials, quantum dots, quantum wires, quantum-bits, etc., are all examples of nanomaterials. Pursuits of methods for preparation, synthesis, characterisation, and detailed examination and prediction of the properties of nanomaterials constitute nanoscience. Special technological benefits from nanoscience demand the exploitation of novel properties at the nanoscale into functionalities for industrial application. The building of functional materials atom-by-atom, molecule-by-molecule, is the challenge for nanotechnology. Since it is a bottom-up approach, it is expected to be devoid of wastage and complexities that accompany prevalent top-down methodologies. The expected efficiency, simplification, local control, and novel applications are reasons for the global attraction for nanotechnology, which is still in embryonic form. However, thanks to concerted efforts around the world, nanoscience is flourishing, and there are reasons to be optimistic about the realisation of the dream of nanotechnology.

By definition, nanoscience is both multi- and inter-disciplinary. Its categorisation is thus non-trivial and intertwined, depending often on whether the emphasis is on the preparation, properties, or functionalities. Based on possible applications, and for the present purposes, fundamental research in nanoscience can roughly be placed in the following, somewhat overlapping, categories:

- manipulation and nanostructuring of materials;
- nanocatalysis;

- nanomagnetism including molecular magnets;
- nanoparticles for drug delivery;
- bio-inspired nanoscience;
- quantum dots, wires, and other nanostructures for electron transport;
- self-assembled monolayers;
- nano-optics; and
- carbon-based technology: fullerenes and carbon nanotubes.

In atom manipulation, scanning probe microscopes (STM, AFM) are used to pull or push atoms with the tip so as to produce desired atomic scale structures. Such an effort is at the heart of tailoring and nanostructuring of materials according to design and functionality. From its initial success in the early nineties in a few laboratories, these techniques are becoming more commonplace, although the method is still confined to very low temperatures, and the ability to obtain reproducible and meaningful results requires substantial expertise. Controlled manipulation of larger entities like nanoparticles is yet another challenge for which novel and innovative techniques are being developed.

The discovery in 1987, by Haruta in Japan, of the high reactivity of Au nanoparticles, has had profound implications for nanocatalysis. The observation that the reactivity of nanoparticles can be so strongly size, structure, element, and environment dependent, that even noble metals can facilitate chemical reactions, raises the possibility of entirely new strategies in the design and selection of catalysts. The further role played by the substrate in supported nanoparticles adds to the challenges and benefits of understanding and developing nanocatalysts.

The lack of symmetry, and the complexity and variety of the local environment in nanoparticles, can also lead to novel magnetic properties, such as the magnetic anisotropies of Co nanoparticles, and enhanced hysteresis, which could have strong technological applications. Arrays of such nanoparticles with well-defined magnetic dipoles also provide examples of systems with controllable magnetic properties (with dominant dipolar coupling). There are also plenty of examples of magnetic behaviour of nanoparticles of materials, which are not magnetic in bulk systems. Similarly, the observation of large magnetic relaxation times of single-molecule magnets, coupled with characteristic steps in their hysteresis curves, offers interesting opportunities for understanding fundamental physics as well as their applicability for data storage and for quantum computing.

Nanoparticles also show promise for other applications, such as as thermo-electric materials, biodegradable polymeric nanoparticles for biomedical applications, nanocomposites (inorganic – organic) for UV and

radar absorption, and nanoparticles for pharmaceutical purposes like drug delivery.

Bio-inspired nanoscience is another area that is ripe with applications. In the biomimetic approach, viruses and other protein cages are used as templates for controlled materials synthesis. The nanoparticles formed by biomineralisation within protein cages offer a fundamentally new approach to produce nanostructured materials with the ability to independently control composition, phase, morphology, size, and size distribution. Furthermore, encapsulation of materials within protein cage architectures allows for the functionalisation of the exterior, tailoring inter-particle interactions, and building designed multi-dimensional arrays.

Nanostructures also allow scientists to manipulate light in ways not previously possible. Metal nanostructures are capable of supporting various plasmon modes, which can result in high local fields and thus in dramatic enhancement of optical response. Such plasmonic nanostructures act as optical nanoantennae, accumulating and building up the electromagnetic energy in small nanometre scale areas. Periodic arrays of metal nanoparticles, arrays of holes in metal films, and metal nanowire meshes may be suitable for tuneable optical responses with frequency, polarisation, and angle-selective enhancements. These materials may also be developed as robust photonic crystals with large and scaleable bandgaps resulting from their negative dielectric permittivity.

Quantum dots are semiconductor nanostructures embedded in another semiconductor. They are perfect examples of systems in which size confinement in all three dimensions leads to discrete energy levels for electron orbits. The separation of the energy levels depends on the size of the dot and can be measured experimentally. Tunnelling of electrons leads to considerable changes in Coulomb energy and single-electron transport dominates transport properties. The interest in quantum dots is driven by the desire to exploit their delta-function-like electronic density of states, and quantum confinement effects in optical devices such as ultra-low threshold semiconductor diode lasers. An important breakthrough came with the development of self-assembled growth procedures, in which quantum dots are created from ultra-thin layers which spontaneously break up as a result of the strain between the substrate and the grown film, and minimisation of their energy leads to the formation of small-scale islands. These self-assembled systems offer enhanced opportunities for understanding fundamental physics and for applications in innovative electronic and optoelectronic devices, and as quantum gates at the centre of a quantum computer. Since the periodic arrays of quantum dots are electrostatically coupled to form a quasi two-dimensional lattice, the inter-dot coupling is tenable, and allows the design of an "artificial crystal."

At the same time, self-assembled monolayers of organic molecules like thiols on gold surfaces continue to be widely used to produce model surfaces with well-defined chemical composition for a variety of applications including biomaterial and biosensor surfaces. Such spontaneous organisation of material through the interaction of non-covalent forces, like van der Waals, hydrogen bonding, electrostatics, etc., has also been found for phosphates and -phosphonates on a number of transition metal oxide surfaces, such as titanium oxide, tantalum oxide, and niobium oxide.

Carbon-based technologies of particular interest are fullerenes and carbon nanotubes. One unique feature of fullerenes is their structural perfection and thus their suitability to be used as building blocks. The cages in these molecules provide further opportunities for absorption, storage, and chemistry. In particular, endohedral fullerenes, which contain a metal atom inside the cage, have been reported to have novel electrical properties. At higher temperatures and pressures,  $C_{60}$  is known to polymerise into a series of one-, two- and three-dimensional structures with electronic properties ranging from semiconducting to metallic, and with a wide range of mechanical properties. Reports of pronounced hardness of three-dimensionally polymerised phases have aroused further technological interest in the fullerenes. Carbon nanotubes, on the other hand, are self-assembling nanostructures and can be metallic or semiconducting depending on their chirality. Of the two structural forms that have been produced, the armchair tubes are known to be metallic, as are one third of the zigzag tubes. The remaining zigzag tubes are semiconducting. Their separation and selective manipulation is thus a challenge. Their high thermal conductivity, optical polarisability, and ballistic transport, together with their structural perfection, make them excellent candidates for various types of applications. Because of their inherent simplicity, they also serve as ideal model systems for systematic studies, so the flurry of activity in this area is not surprising.

## Nanoscience and Nanotechnology in Sweden

As in other countries, research efforts in the area of nanoscience have increasing importance in most institutions. At Lund and Linköping universities, there are centres dedicated to multi-disciplinary work in nanoscience. A similar centre has recently been created at Uppsala University. At Chalmers and at Göteborg University, nanoscience has become a major component of the activities of several research groups, which had previously engaged in work in the related areas of surface and cluster physics. Indeed, high quality research in nanoscience is being carried out to varying extents in almost all universities in Sweden. Below, is a summary of some of the Research Council-

supported ongoing work at Swedish universities. Note that the summary below does not include the important areas of spintronics and quantum computing, since they are placed under the topical section of activities in semiconductors and superconductors. Some of the topics included under nanomagnetism may also be found under the topical area of magnetism.

### Nanoscale Manipulation and Imaging

In collaborative work, Krister Svensson (Solid State Physics, CTH/GU), Eva Olsson (Microscopy and Microanalysis, CTH/GU), and Håkan Olin, currently at Mid Sweden University, have recently provided an answer to the issue of manipulation of nanoparticles and clusters containing thousands of atoms for which SPM is not the proper technique. By using carbon nanotubes as nanopipettes, Svensson *et al.* showed that electromigration forces conspire in the transport of material from one point to another. This outstanding work has benefited greatly from the patented instrument that the same group of scientists had developed earlier, in which a movable STM probe was incorporated into a transmission electron microscope (TEM). The big advantage of this instrument is that *in situ* manipulation of nanoscale material, and measurement of its electrical properties, can be done simultaneously with imaging. It is to be noted that Håkan Olin pioneered the development of the TEM-STM method, and received several innovation awards for this development. Many of his scientific contributions have been breakthroughs in the field of nanoscience and/or nanotechnology and have made an impact on the field. Interesting are the discovery of quantised conductance in Bi nanowires, the first images of a point contact, interaction between atoms on a Cu surface, construction of a room temperature SET, a nanoelectromechanical switch and nanotube pipettes, etc. This research effort of Olin, Svensson, Olsson, and their co-workers is outstanding and world-class. Already the application of the technique to examine transport in Bi nanowires and plastic deformation of Si wafers and nanowires has provided microscopic insights into the associated phenomena – for the first time. The future plans of Olin, Svensson, and Olsson, in their respective universities, to develop a fundamental understanding of electrical and mechanical properties of nanowires, are promising.

In this same general area of research, painstaking and much-needed developments in one of the most popular present-day techniques – Atomic Force Microscopy (AFM) – were carried out by Ragnar Erlandsson at Linköping University. After participating in pioneering work at IBM Almaden Research Center, Erlandsson returned to Sweden and chose to build AFM/STM laboratory from scratch in Linköping. With the home-made system, his group was able to obtain true atomic resolution and show

for the first time in their investigation of the  $7\times 7$  reconstruction of Si(111) the contrast effects among similar atoms on the surface. His group also developed the force feedback system, which allows the measurement of tip-sample forces with extreme sensitivity. Despite the success of the group in bringing about profound developments of the AFM, Erlandsson has quit research, and states in the written document the lack of sustained funding of his academic position as the reason. This is perhaps one of the starkest examples of the negative impact of the “25 – 50% professor” that does not foster long-term and serious efforts in instrument and technique development.

In related theoretical work, Mats Persson (Materials and Surface Theory) at Chalmers University has pursued an outstanding research activity in developing an understanding of the manipulation and characterisation of atoms at surfaces by scanning probe techniques. In the formulation of interesting problems, Persson has chosen to work closely with leading experimental groups to great effect. Persson’s group is sought by leading experimentalist, such as Wilson Ho and Karl Heinz Rieder, for theoretical support for their experimental observations. The approach has been to develop new physical concepts by using DFT calculations in combination with simple model Hamiltonians. Their modelling of electron tunnelling in a scanning tunnelling microscope junction involved new theory and computational codes for the calculation of the efficiency of vibrational excitations in inelastic electron tunnelling. In this way, new insights have been gained into surface state mediated adsorbate – desorbate interaction, single-molecule vibrational spectroscopy and microscopy, single-molecule chemistry, resonant electronic states in magnetic and non-magnetic adatom nanostructures, and charging of single atoms.

### Nanocatalysis

Arne Rosén’s group (Molecular Physics, CTH) has developed sophisticated techniques including second-harmonic generation, to examine the chemical reactivity of free clusters and the optical activity of supported clusters. Future plans include the use of sum-frequency generation, which should provide far more specific spectroscopic information. In the group, Mats Andersson’s excellent experimental work on the chemical reactivity of 5 – 1550 atom metal clusters in vacuum provides a very nice cross-link to conventional surface science on extended surfaces and to “real” catalysts. The investigations of CO on Cu clusters demonstrated striking behavioural differences as a function of temperature – a very difficult parameter to control or measure in naked cluster experiments – and size. The size dependence displayed a shell structure. As in several places in Sweden, experimental

groups have excellent overlap with theorists in the group. Individuals in Rosén's group also engage in theoretical calculations using a variety of techniques. Collectively, this group is carrying out excellent work in the area of nanocatalysis. Also at CTH, another excellent surface science group is that of Bengt Kasemo's, whose present activities include nanocatalysis. Their recent work with J. Libuda *et al.* at the Fritz Haber Institute in Berlin on the fabrication of a model catalyst, using a range of surface science techniques and DFT calculations, is at the cutting edge of the field. Bo Hellsing, in the Solid State Physics group (headed by Lars Walldén) at Chalmers, is also engaging in DFT calculations of the reactivity of nanoparticles, in collaboration with Risto Nieminen's group in Helsinki. The Expert Panel would like to encourage Hellsing to pursue these calculations, particularly in collaboration with local experimentalists in the groups of Rosén, Kasemo, and Walldén.

### Nanomagnetism

In the Solid State Physics group (headed by Lars Walldén) at Chalmers, the main activities are concentrated on the study and development of nanostructured magnetic materials with novel properties. Very good work has been reported on the static and dynamic properties of magnetic domains, the entities linking the basic physical properties of a material to its macroscopic properties. On the applied side, the aim is to find a prototype of an ultra-high density memory and a non-volatile random access memory (MRAM). Börje Johansson and co-workers (Applied Materials Physics, KTH) are engaged in theoretical studies of magnetism in low-dimensional systems, specifically metallic nanowires suspended between leads. Using first-principles computational methods, magnetic phenomena were investigated in nanowires of 4d and 5d transition metals, i.e., metals that are normally nonmagnetic. An important result of this internationally competitive project is that many of these metals are predicted to be magnetic, or more accurately super paramagnetic, in nanowire form. The Materials Chemistry group (headed by Mamoun Muhammed), also at KTH, has undertaken an excellent, major project to develop multi-functional nanoparticles to be used in several biomedical applications, including MRI, tissue engineering, therapeutics, hypothermia, *in situ* monitoring, diagnostics, etc., and superparamagnetic nanoparticles of different composition have been prepared. Muhammed's group is among the first to develop nanoparticles with magnetisation very close to the theoretical value, which is superior to comparable commercially available materials. Other nano-objects, including nanorods, nanotubes, and nanowires, have been studied.

Three very promising contributions within this contemporary area are performed by the young and apparently very talented researchers: Stephanie Reimann (Mathematical Physics, LU), Tatiana Makarova (Experimental Physics, UmU), and Carlo Canali (Condensed Matter Physics, Kalmar University). Reimann focuses on theoretical studies of electronic and spin structures of dot lattices. Surprisingly, a rich but systematic magnetic behaviour of square quantum dot lattices was observed. Dots with half-filled electronic shells form antiferromagnetic insulators and are even more persistent against metallisation than lattices built of quantum dots with closed shells. Other work with much impact was the discovery of broken spin symmetries in quantum dots, both within the spin density functional approach and exact diagonalisation studies. Makarova has made the un-expected discovery of ferromagnetism in  $C_{60}$ . In contrast to other organic magnets, the Curie temperature is well above room temperature. Although the experiments have been repeated with identical results in several laboratories worldwide, “magnetic carbon” is still a very controversial subject, since the paired electrons in the C atom are very unlikely to produce a net magnetic moment.

Recent experiments have also shown that local ferromagnetism can be induced in  $C_{60}$  by laser- and electron-beam irradiation. Creation of such magnetic patterns in the micro- or nanometre scale can have huge technological implications and potential application in spintronics, optics, and quantum computing. Makarova and co-workers are trying to find optimum conditions for high-pressure production of magnetic carbon, and inexpensive ways to produce such materials in bulk amounts; this is excellent work. Canali’s research interests centre primarily on quantum many-body physics in low-dimensional systems, the theory of disordered systems and the field of nanophysics. Recently, the interest in quantum magnetism and the study of elementary excitations in magnetic systems have had a strong revival, in connection with itinerant magnetism and spin-dependent tunnelling transport in ferromagnetic metal nanoparticles and nanowires. The most important results are the discovery of unexpectedly large fluctuations of the nanoparticles magnetic anisotropy energy, abrupt jumps in the quasiparticle excitation energies at the classical switching field, and the crucial role played by the orbital magnetic moment to the  $g$ -tensor in metallic nanograins. The future research work will focus primarily on quantum magnetism and spintronics in nanostructured-systems, also excellent work.

By altering the interaction potential in magnetic heterostructures, the effective dimensionality can be tailored. Björgvin Hjörvarsson (Materials Physics) at Uppsala University has accomplished this by selective *in situ* “doping” by hydrogen, enabling the switching and tuning of the interaction

potential, changing from antiferromagnetic (negative) to ferromagnetic (positive) interlayer coupling. Reversible tuning of the magnetic exchange coupling in Fe/V (001) superlattices was established. This approach opened up completely new routes to address the influence of exchange interactions on the dimensionality of the magnetic fluctuations in magnetic heterostructures. A new class of magnetoresistive semiconductors, namely the magnetic rare earth hydrides, was discovered as a result of this excellent research activity. These materials exhibit large magnetoresistance at low temperatures. Also in Uppsala, Per Nordblad and others (Solid State Physics) study arrays of micron- and sub-micron-sized magnetic elements, defined by electron lithography. This excellent work has its emphasis on the equilibrium magnetic microstructure of the demagnetised state, as well as the nucleation process of domain walls and the transient domain configurations appearing during magnetic switching. The current work is focused on permalloy elements and epitaxial multi-layers. Moreover, at UU, the Surface Physics group (Nils Mårtensson) has a programme concentrated on composite magnetic nanostructured materials tuned in terms of elemental composition and approaching atomic size in one or more dimensions. Depending on the specific sample, the techniques of X-ray Magnetic Circular Dichroism (XMCD), X-ray Resonant Magnetic Scattering (XRMS), Extended X-ray Absorption Fine Structure (EXAFS), and Dichroism X-ray Photoemission Spectroscopy (DXPS) have been applied. They have a wealth of experience in the characterisation of ultra-thin magnetic film systems, multi-layers, and nanostructures. In particular, their interests have centred on the spectroscopic techniques, magnetic anisotropy, and, more recently, exchange bias.

Finally, within this subarea, a very impressive and excellent project in Kajsa Uvdal's group (Applied Physics and Sensor Science and Molecular Physics, LiU) is centred on developing magnetic nanoparticles ( $Gd_2O_3$ ) as a magnetic resonance imaging contrast agent. The long-term goal of this project is to develop cell-level imaging techniques, which would have potentially important applications in the early detection of brain tumours. This is an example of a successful research project between Faculties – from the physical sciences and from medicine. Uvdal intends to tailor novel magnetic properties of nanoparticles for MRI contrast enhancement.

### Multi-Functional Nanoparticles

Mamoun Muhammed's Materials Chemistry group (KTH) works on developing new methods to synthesise nanoparticles and nanostructured materials. The long-term motivation for the research is to make functional materials tailored for applications, for example, in medicine for magnetic resonance imaging and in targeted drug delivery. The group also processes

nanostructured materials, which are metals, semiconductors, ceramics, or polymers. Of great interest is the development of nanoparticles to be used in MRI, tissue engineering, therapeutics, etc. Muhammed's group is among the first to develop methods for the fabrication of nanostructured thermoelectric materials. Their work demonstrating significant reduction of thermal conductivity as result of nanostructuring is also an important contribution to the field. The fabrication of several doped skutterudite thermo-electric materials is also an excellent achievement. An ongoing project is the development of drug-carrying particles *in vitro* for the purpose of targeted delivery of drugs *in vivo*. Promising multi-functional materials, consisting of biodegradable polymeric matrix containing temperature-sensitive polymer-drug nanoparticle complexes have been synthesised. Given the overlapping interests and applications, the Expert Panel envisions further synergy in joint activities of the Osamu Terasaki (Inorganic Chemistry, SU) group in direct imaging with electron microscopy of the partially ordered materials prepared by Muhammed's group. The work of Terasaki on structural characterisation of mesoporous materials is clearly at the forefront of this research area worldwide. Over the years, this investigator has assembled an impressive set of collaborations with other internationally renowned materials chemists. A major area of current and proposed future research is the synthesis of nanocluster-arrays within the cavities of porous zeolites and mesoporous crystals. The materials are expected to exhibit important electronic and optical properties resulting from the quantum mechanical coupling of clusters arranged on periodic structures. By far the most important contribution of Terasaki has been the development of electron microscopy methods for the quantitative microscopic structure determination of both the mesoporous crystals and the nanoscale clusters they contain. The structure determination by him involves examples of tour-de-force experimental ingenuity. Terasaki's work is clearly excellent/outstanding.

Hans Siegbahn's group (Electron Spectroscopy and Molecular Surface Physics) at Uppsala University has developed novel tools for investigating the electronic structure and energy matching for molecules at nanostructured surfaces, molecular structures of these molecular assemblies, as well as dynamic processes (charge redistributions and charge injections) between the different materials. Some of this work is in collaboration with Per Uvdal (Chemical Surface Physics) at Lund University. The success in the use of future advanced nanostructured materials partly depends on the detailed understanding and the possibility to control the structure – function relationship within surfaces and interfaces. The very good activity of Siegbahn in this field is based on studies of nanostructured-nanocrystalline oxide films and is focused on issues related to energy conversion, energy storage,

and displays. In this highly interdisciplinary research, Siegbahn's group has contributed to the understanding of charge separation at nanostructured surfaces, charge transport in nanostructured systems, and application to practical solar cell devices. Advances have also been made in the understanding of the interfacial electronic structure of molecularly modified nanostructured networks. Charge transfer dynamics related to the photo-conversion process was studied, using resonant photoelectron spectroscopy allowing charge redistributions occurring within the femtosecond time-regime to be detected. Future studies in molecularly modified nanostructured materials would explore how adsorbed molecules (co-adsorbers) influence the charge transfer kinetics and energetics and, subsequently, the conversion efficiencies of dye-sensitised solar cells. New designs, such as coating of nanoparticles with a thin blocking layer of non-conducting oxide materials (forming "coreshell" type materials), will be tried to reduce the amount of photocurrent losses in the photoconversion system. The electronic and geometric properties of the different constituents, especially at the interfacial regions, will be characterised in collaboration with several groups.

On the theoretical aspects of nanoscale materials, Bengt Lundqvist and his group (Materials and Surface Theory) at CTH have, through the decades, led the developments and applications of state-of-the-art theoretical and computational techniques to complex problems on surfaces and nanostructures. Recent pioneering work by Lundqvist and Per Hyldgaard on a development of DFT-based calculations of out-of-equilibrium transport and dynamics extends microscopic theory, and shows a breakdown of Landauer-Büttiker transport, provides a consistent transport description, and gives the thermal conductivity across silicon-carbide contacts. Through its usage, a robust nanosized transistor effect in nanotube resonant-tunnelling heterostructure has been predicted, and is a stimulus for the NanoIC patent. Outstanding work by Lundqvist and Hyldgaard on understanding the ubiquitous van der Waals (vdW) interaction has been vital for development of *in situ* nanostructure growth and integration. The vdW interaction is generally weak, but defining, for the strength of interactions in, *e.g.*, carbon nanostructures on growth substrates. The Chalmers/Rutgers development of a new density functional gives an extension of microscopic theory that is critically needed to understand sparse-matter problems. The underlying traditional DFT implementations raise worrying issues, however. This and refined non-local correlations call for a deepened analysis, in parallel with massive applications of vdW-DF to all kinds of sparse systems. This is the essence of some of the work proposed for the future by the group.

### Bio-Inspired nanoscience

One promising aspect of Ingemar Lundström's research (Sensor Science and Molecular Physics) in bio-inspired nanoscience at Linköping University is its multidisciplinary nature and extensive collaboration with faculty in the medical sciences. The "twinning" of graduate students from different disciplines in collaborative work is helping further institutionalise cross-disciplinary activities. In connection with their extensive excellent activities in the area, the group has developed a reliable protocol for the preparation of molecular gradients on gold, using a cross-diffusion methodology, which has been utilised to optimise properties of thin films for biomaterials and biosensing applications. Furthermore, they have created a platform for the use of helix-loop-helix polypeptides in optical, fluorescence-based, biosensing.

Per Nordblad's (Solid State Physics), Uppsala University, excellent effort in biomagnetism aims at making use of the knowledge gained in the nanomagnetic project and to apply it to the area of nanobiotechnology. The objective is to exploit nanomagnetism, by using externally operable sub-micron-sized magnetic elements in combination with colloidal magnetic nanoparticles. The multi-disciplinary nature of this work is exciting. The appointment of Maria Strömme – from Solid State Physics division (headed by Claes-Göran Granqvist), in which Nordblad's group is a subgroup – as the new Chair in Nanotechnology at Uppsala University, is very positive. This is expected to facilitate cross-disciplinary research, particularly in the applications of decades of technical expertise in the fabrication of nanomaterials to problems in pharmaceuticals. Future research is expected to understand and exploit nanoscale properties of functional polymers for biomedical applications. This combination of basic and applied science sounds very promising.

The development of nanoimprint lithography in Lars Samuelson's group (Solid State Physics) at Lund University, has paved the way for the assembly of novel nanodevices, for controlled formation of nanowire arrays, and for life-science applications. Collaborative work with faculty in the life sciences has been very fruitful for research applications, as well as in the training of students.

### Nano-Optics

Very good work on material coatings in Claes-Göran Granqvist's group (Solid State Physics) at Uppsala University, has turned to the production of metal or metal oxide nanoparticles, with narrow size distribution, using advanced gas deposition technology. Nanoparticles thus fabricated are targeted for application in semiconductor chemical sensors, and for those based on electromagnetic fluctuations and dc resistance. Excellent synergy

between experimental and theoretical work in the group, including efforts of E. Wäckelgård, has led to better understanding of the size-optical property relationship and optimisation of the spectral selectivity of the nanoparticles fabricated by Granqvist's group. This collaborative work has also established the importance of Ni-alumina nanocomposite, from chemical solution synthesis, as spectrally selective solar absorbing surface.

The Condensed Matter Physics group of Lars Börjesson at Chalmers University of Technology (CTH) is engaged in excellent/outstanding work in applications of nano-optics based on the resonantly enhanced near-field produced by surface plasmons and in the development of nanoscopic biosensors. Issues addressed include theoretical and experimental foundation for the single-molecule Surface-Enhanced Raman Scattering (SERS) phenomenon, and optimisation and design of plasmonic properties using nanolithography. Their pioneering work in nano-optics has been rewarded by a partnership in the EU Network of Excellence, PHOREMOST, beginning in January 2005. Among notable achievements of Börjesson's group is the first vibrational spectroscopy measurement of single-biological macromolecules (Hb, using SERS) and an explanation for the single-molecule SERS phenomenon, in terms of electromagnetic "hot spots" at the junction between resonant nanoparticles. Mikael Käll *et al.*'s work in the group has led to the discovery of tuneable SP resonances in gold, nanorings, and nanoholes. The group is also credited with the first demonstration of optical manipulation of plasmonic nanoparticles in solution. Furthermore, they have developed an ultra-sensitive nanoparticle sensor for DNA hybridisation detection.

Peter Johansson (Solid State Physics) at Örebro University, conducts very good theoretical calculations of the electromagnetic response of nanometre-sized systems by solving classical equations in complex geometries. He has collaborations with some of the leading experimentalists in the field and his work facilitates interpretation of experimental data. For example, his theoretical model for calculations of SERS intensities, in which electromagnetic enhancement effects and vibrational dynamics of the molecule are treated on an equal footing, was able to account for the many orders of magnitude enhancement in the Raman scattering cross-section of molecules adsorbed on metallic nanoparticles, in good agreement with experimental data. Perhaps even better known is the work on light emission from STM measurements for an alkali overlayer on Cu(III), in which the interplay between electromagnetic enhancement effects and quantum well states of the system lead to emission, even when it is otherwise forbidden. The explanation was attributed to a hot-hole and/or hot-electron cascade near the tip. Johansson's future work will continue in the area of near-field optics, with the focus on interactions between electromagnetic radiation and molecules

adsorbed on nanoparticles. Some work is also planned in magnetoptics. Most of the work will continue to be in collaboration with experimentalists and also other theorists (in Lund), a good strategy, indeed. Johansson's work is very relevant to the present day scene in nano-optics and nanoscale science, as such. His calculations are phenomenological, and their validity comes from their relevance to state-of-the-art experiments.

### Quantum Dots, Quantum Wires, and Other Semiconductor Nanostructures

Bo Monemar and Per Olof Holtz's group (Materials Science) at Linköping University is engaged in excellent work in quantum dots, wires, and other semiconductor nanostructures. One of their highlights is the control of the charge state in quantum dots through purely optical means. The group was one of the first to establish the relative role of capture/relaxation processes of carriers and competing Auger processes, and to observe indirect-direct transitions in Si/Ge quantum dots. They have also used quantum dots as probes to identify nearby impurities. The work on coupled quantum wire LED's has shown exciton tunnelling up to room temperature, and the role of triaxial strain in lattice-mismatched quantum wires has been investigated. Fundamental issues in spin interactions and mechanisms controlling growth, and structural designing of MnSe and CdMnSe nanostructures, are being examined systematically by Weimin Chen (Materials Science) at Linköping University, in internationally recognised work. Future efforts of the group include developing an understanding of the electronic structure of single quantum dots, and identification of recombination processes in novel systems, e.g., nitride and SiGe quantum dots. The effect of magnetic fields on transport properties will be examined with the dot employed as a probe. Electroabsorption modulation of quantum wires will also be investigated, using a combination of the quantum confined Stark effect (QCSE) and phase-space absorption quenching (PAQ).

Very good theoretical work based on DFT by Karl-Fredrik Berggren and Irina Yakimenko of the Theory and Modelling group at Linköping University shows that the dissipative processes in the quantum cellular automata (QCA) play a decisive role in the propagation of polarisation along the array of quantum dots. Imperfections may impair the switching properties of the semiconductor-based QCA. The spin-polarised states were shown to play a role in the determination of the conductance of quantum dots, quantum point contacts (QPCs) and their arrays, and in quantum wires. Future work of the group includes more accurate and realistic theoretical modelling of the low-dimensional semiconductor systems, in particular quantum wires, quantum point contacts, and quantum dots. The study will include electronic structures, transport phenomena, effects of electron – electron

interactions, spin states and nanomagnetism, non-collinear magnetism, and modelling and functionality of nanodevices for quantum information processing. A proposed study of conductance anomalies in the quantum wires, and spin-injection in lateral p-n junctions and the shell structures in GaAs and Si nanorods, sound promising. Igor Zozoulenko (Mesoscopic Physics and Nanoelectronics, at Campus Norrköping) has carried out very good theoretical work on developing an understanding of magneto-conductance and electron dynamics in ballistic chaotic and regular quantum dots. He is developing a quantum mechanical description of magneto-transport in arrays of quantum antidots.

Stephanie Reimann (Mathematical Physics, at Lund University) engages in excellent theoretical studies of single quantum dots, as well as their periodic arrays with on-going collaborations with Matti Manninen in Finland. An intriguing finding is that dots with half-filled electronic shells form antiferromagnetic insulators and are more persistent against metallisation than lattices, built of quantum dots with closed shells. In her recent work on vortices in finite quantal systems, rotation of trapped particles (both bosons and fermions) with a repulsive interaction is shown to lead to vortex formation. These results may have consequences for physics in the fractional quantum Hall regime, and also for rotating Bose–Einstein condensates. This work is also related to their previous discovery of broken symmetries and localisation at the edge of quantum dots in strong magnetic fields.

Also notable is the discovery of broken spin symmetries in quantum dots, which shows that the ground states of quantum rings have an internal structure that is antiferromagnet-like, with particles localised along the quantum ring. Similar broken spin symmetries turned out to be important for the magnetism in square lattices with quantum dots. For quantum dots in strong magnetic fields, Reimann has examined the stability of vortex formation in the presence of irregularities in confinement or impurities. As in rotating Bose condensates in quantum dots, a flattening of the potential well may lead to the occurrence of “giant” or multiply quantised vortices. These studies are performed in collaboration with the group of Risto Nieminen and Martti Puska (Helsinki University of Technology, Finland).

### Self-Assembled Monolayers (SAM)

In the fascinating area of SAM, investigations in Ingemar Lundström's group (Sensor Science and Molecular Physics, Linköping University) of Tyrosine and DOPA derivatives adsorbed on gold surfaces show that the self-assembled layer is covalently bonded to the substrate and laterally stabilised, through hydrogen bonds. Their NEXAFS measurements have provided valuable information about orientational effects correlated with the aromatic

rings and locations of the peptide bonds. Their extensive temperature programmed studies with mass spectrometry and infrared spectroscopy, in the temperature interval 77 – 500K, have provided a comprehensive understanding of the structure and temperature-driven phase behaviour of oligo (ethylene glycol) self-assembled monolayers on gold. These studies provide a molecular understanding of the basic interactions between oligonucleotides and planar gold surfaces. They have utilised the concept of folding as a generic tool, to build novel nanoparticle assemblies – “a nanoparticle Lego”.

SAM of various molecules has also been studied with success by Lars Johansson and Ellen Moons (Materials Physics, Karlstad University) with high-resolution core-level spectroscopy at MAX-lab. New information about bonding and interactions has been obtained.

One of the most internationally recognised groups in the field of nanotechnology is the Solid State Physics of Lars Samuelson, at Lund University. Within the last five years, they have established one of the leading laboratories worldwide in research on semiconductor nanowires. In the area of quantum devices based on designed nanoparticles, the group has pioneered the use of aerosol techniques for the formation of highly ideal metallic and semiconductor nanoparticles, including core-shell particles designed for device functionality. Samuelson *et al.* have developed a method for Ångström-level control in the assembly of quantum devices, using the atomic force microscope (AFM) for highly accurate manipulation of nanoparticles. Samuelson *et al.* have also developed the field of self-assembly of QD's – and they were the first to obtain high-resolution images. Further insights into their observation of luminescence of single self-assembled quantum dots and theoretical modelling provided their few-electron states. The effects of multiple charging were studied by electrical and optical means. STM-induced luminescence was used to correlate structural and optical properties of single QD's. From correlation spectroscopy, anti-bunching properties, important for quantum optics, were extracted. Samuelson and co-workers in the field of quantum dot ratchets, in which electron-wave interference is used to create a non-linear voltage response, have carried out pioneering work. Tunnelling ratchets, which resemble the energy-sorting task of a Maxwell's demon, were also studied. Furthermore, Samuelson's group was the first to demonstrate size- and site-controlled formation of nanowires and was also the first to demonstrate atomically abrupt and perfect heterointerfaces in nanowires. Self-assembly of nanowires has also been employed to produce nanoelectronic devices. Collaborative work has led to the creation of 3D nanowire structures in the form of nanotrees. Insightful studies of the internal atomic structure inside nanowires, as well as the mechanisms of nanowire formation, have also been investigated by this impressive group

of researchers. The research activities in Samuelson's group are outstanding, and the ideas and concepts very innovative. The research is multi-disciplinary and spans a variety of topics in nanowires, ranging from their growth, quantum physics in nanowires, nanowire devices, and finally the use of nanowires in life science applications.

### Fullerenes and Carbon Nanotubes

Groundbreaking work by Eleanor Campbell and co-workers (Atomic Physics, CTH/GU) has led to the development of a low-energy ion implantation technique for the production of endohedral fullerenes ( $C_{60}$  molecules containing a metal atom inside the carbon cage). Because of their high stability and symmetry, endohedral  $C_{60}$  molecules are particularly interesting for both fundamental research and potential applications. Excellent work by the group has already unveiled the dynamical properties of  $Li/C_{60}$  and also determined energy coupling dynamics in isolated fullerenes and endohedral fullerenes using ultrashort-pulsed lasers. They are now developing a new ion source for the implantation of non-alkali metals, such as Al and La. The focus is on understanding the trends in the dynamical and electronic properties of various endohedral fullerenes in gas phase, and in thin films under varying atmospheric conditions. The application of the technique to implantation in CNT's, with the aim of producing nanotubes with the desired property at a specific location on a silicon chip, using CMOS compatible methods, looks very promising. Proposed work on nanomechanics, which involves optimised production and characterisation of the dynamical properties of the carbon nanotube relays and of fullerenes inside nanotubes "peashooter", is also appealing. The Panel was also encouraged by the collaborative work that Campbell has with scientists locally, nationally, and globally. It is encouraging to see the synergistic interactions with Yu Zhang (Materials Chemistry) at KTH, in this connection.

Excellent theoretical work on the operational characteristics of nano-electromechanical devices, such as the carbon-nanotube-based three-terminal nanorelay, by Jari Kinaret and Mats Jonson (Condensed Matter Theory, CTH), shows that short range and van der Waals forces have a significant impact on the characteristics of the relay, and may introduce design constraints. Theoretical analysis of the high frequency properties of the device has demonstrated its potential for a number of applications, such as tuneable band pass filter, voltage controlled oscillator, memory element, etc. in the microwave range. The Expert Panel was impressed by the synergy between the theoretical research of Kinaret and Jonson, and the experimental work in Campbell's group. In addition, the Molecular Physics group (Arne Rosén and others) is engaged in excellent systematic

fundamental studies of carbon nanotubes (CNT), using a range of experimental and theoretical techniques, and focusing on issues as varied as their thermal properties, collision dynamics, chiral-selective manipulation, as well as their growth mechanisms. Together with the experimental group of Peter Eklund, Pennsylvania State University, USA, Rosén *et al.* were the first to show that the electrical properties of CNT's were strongly affected by collisions with inert gases, indicating the importance of collision-induced phonon excitation and/or indentation of the CNT. On the critical issue of chiral-selective manipulation and separation of CNT's, Rosén's group has proposed a chemical method for separating zigzag from armchair nanotubes, based on nanotube functionalisation, whereby hydrocarbons are attached to the nanotube ends via a link heteroatom. Proposed collaboration with Eleanor Campbell should aid experimental validation of the theoretical predictions. In related very good work, molecular dynamics simulations carried out by Kim Bolten in Rosén's group have identified the roles that catalytic metal clusters, the solvents, and their mutual local environments play in the growth of CNT's. These insightful microscopic results point to the importance of accurate description of the electronic motion and dynamics of the system through more accurate techniques like DFT, which will be pursued by the group in the future.

The pioneering work of Håkan Olin (who has recently moved from CTH to Mid Sweden University) together with Krister Svensson and Eva Olsson, CTH, on CNT-based nanopipettes needs to be mentioned again in this subsection, as it is a remarkable application in manipulating matter at the nanoscale with carbon based technology.

The field emission of electrons from the tip of carbon nanotubes has been targeted for low energy illumination, and as an extremely coherent and bright electron source. If successful, it could be one of the first commercial applications for CNT's. Reine Wallenberg (Materials Chemistry) at Lund University is engaged in a novel research effort on optimising field emission of electrons from carbon nanotubes (CNT's), for the purpose of developing bright electron sources. They have successfully demonstrated field emission from single CNT's. The proposed future research is on obtaining field emission from nanoscale whiskers. The research will focus on fundamental studies elucidating the parameters, which control whisker length, diameter, composition, and surface density. Wallenberg's group has also focused on several device applications of nanowires, such as a resonant tunnelling diode, which the group reported in 2002, a working single-electron transistor reported in 2003, followed by that of nanotrees in 2004. These applications were carried out in collaboration with the Solid State Physics group of Lars Samuelson at Lund University.

Bertil Sundqvist's group (Experimental Physics) at Umeå University has, for over a decade, been engaged in very good/excellent work on the physical properties of fullerenes and other carbon-based nanostructured solids under variations of pressure and temperature. Their studies of the thermo-physical properties of molecular  $C_{60}$  and  $C_{70}$  under extreme conditions has helped map structural-phase diagrams for the systems, which were reproduced much later by neutron and X-ray scattering measurements. They have also pioneered the high-pressure-induced polymerisation of single crystal  $C_{60}$  into one- and two-dimensional phases, as well as long-range ordered polymeric form of pure  $C_{70}$ . Among the interesting observed electrical, thermal and magnetic properties of these materials was the unexpected discovery of ferromagnetism in  $C_{60}$  (discussed earlier). Work is in progress to understand the formation and structural evolution of these fascinating materials under pressure. Further structural studies are also in progress, using a new Scanning Probe Microscope, on two-dimensional structural phases of monoclinic  $Na_4C_{60}$  and tetragonal  $Li_4C_{60}$ , to understand their surprisingly large structural difference. The work of Sundqvist *et al.* in the electrical transport properties of CNT under high pressure and at low temperature shows differences in the effective dimensionalities in pristine and "purified" samples, and calls for more microscopic understanding of the relationship between structure and property. The extension of high pressures to examine the so-called "peapods", nanotubes filled with fullerenes, and fullerene polymerisation under extreme confinement conditions, is promising as it might point to a controlled way of producing material with interesting novel properties. The availability of the new SPM would facilitate the work and allow the possibility of manipulating tubes and tube arrays or compounds on a small scale. The efforts by Alexandr Talyzin *et al.* to produce nanostructured carbon material directly from molecular hydrocarbons by thermal decomposition under extreme conditions, is also promising.

Joseph Nordgren (Soft X-ray Physics) at Uppsala University was one of the first to apply RIXS to characterise the femtosecond time scale of dynamic vibronic coupling in  $C_{60}$ . As a by-product, ideas about the scattering process itself were further developed, leading to the scattering-duration time concept now widely used. They were able to characterise the Ti- $C_{60}$  chemical bond and show that, contrary to common belief, stable early transition metal fullerides do exist. One of the most studied fullerides is  $K_3C_{60}$ , a highly correlated material that becomes superconducting at low temperatures. Using photoemission and RIXS, Nordgren *et al.* showed that the electronic structure in the metallic bulk differs significantly from the insulating surface. The work of this group is excellent.

Sven Stafström of the Theory and Modelling group at Linköping University has carried out excellent studies of charge transport and electric contact problems of conjugated carbon-based systems, such as fullerenes and CNT. These studies involve first-principles density-functional theory for basic electronic and structural properties, time-dependent Schrödinger equation for studies of electron dynamics, Landau theory for transport in molecular wire systems, and finite size scaling for studies of electron localisation. The theoretical and computational work by Stafström *et al.* has led to the introduction of fullerene-like carbon nitrides; in particular, the molecule  $C_{48}N_{12}$  has been predicted to have interesting properties. Jörgen Rammer's (Theoretical Physics, Umeå University) preliminary theoretical work in understanding thermoelectric phenomena in quantum nanostructures looks promising. The main goal of the investigation is the identification of the physical mechanism which drives the magnetic transition in pure carbon. Using quantum chemical *abinitio* methods, a theoretical model was developed, which allows interpretation of most of the available experimental data on the magnetism of polymerised fullerenes.

## Future Perspectives

In the short span of five years, “nano” has become a buzzword and nanoscience has become intertwined with nanotechnology. Funding agencies have looked favourably at projects that pertain to nanoscience and expect to lead to nanotechnology. Researchers have found ways to emphasise the nano-ness in their on-going activities, and to indulge in activities that are more overtly nano. Popular media has also picked up on the trend, and articles on the perceived promises and perils of nanotechnology and their social and political impact are easy to find. To some, nanotechnology is the solution to all evils in society, and its dawning will be the path to utopia, as if science and technology alone possess this power. To others, there is much to fear, and the belief that uncontrolled developments in this field will ultimately lead to the collapse of our planet. Whatever the perspective, it is clear that “nano” has caught the imagination of the world at large. The question now is: can we, scientist and engineers, deliver?

The answer is a qualified “yes.” Already, efforts in nanoscience have taken us in new directions. First, there is the recognition that synergistic activity among scientists, engineers, and other scholars, can lead to breakthroughs in scientific discovery that may not otherwise be possible. Second, for such multi-disciplinary activity to be successful, knowledge acquisition and its implementation have to proceed from a number of different platforms and perspectives leading to a more “holistic” approach. Third, and perhaps

most importantly, nanoscience, being a bottom-up approach, provides opportunities for invoking new methodologies and new paradigms for knowledge acquisition and discovery. While conventional methods are appropriate for understanding characteristics of systems at macroscopic scales, it is at the microscopic scales that novelty in properties demands novel approaches for their understanding and control. Theory, modelling, and experiments have thus become equal partners in the acquisition of microscopic information, and together they are establishing a framework for understanding the characteristics of novel functional materials. Such a framework opens the way for inclusion and extension of the work to areas as varied as artificial intelligence, on the one hand, and biology, on the other, making research in nanoscience and nanotechnology more inclusive. It also invites non-conventional thinking and innovative approaches, for the benefit of all. The promise of nanoscience is thus to create a cadre of scientists who are able to use their training in condensed matter physics to understand and control the properties of biological functional material for health, environment, and engineering applications. This is a challenge that the world seems to have accepted, as have scientists in Sweden. It is a challenge, which if brought to fruition, has the capability to bring about significant changes in our lives. From drug delivery, to cancer diagnosis, to quantum computers, to miniature magnetic storage devices, to cleaner environments, to more affordable catalysts, they all affect our lives and can bring about changes in the way we live and do business. For these reasons and more, research in nanoscience has to be taken seriously. The general message from the survey of CMP in Sweden is that nanoscience has already established itself as the upcoming research area, and has done so through integration, and as a result of a natural evolution of existing frameworks for scientific discovery. These are positive signs and, undoubtedly, scientists in Sweden are on their way to making an impact in this promising field, just as they have done in areas like surface physics.

## Magnetism and Spintronics

### International Perspective

Within the last two decades magnetism, and especially spintronics, has emerged worldwide as a highly topical subfield of condensed matter physics. The theoretical advances and the strong involvement of magnetism in all branches of technological development make this discipline one of the most relevant areas of current research. As industry seeks faster, cheaper

and higher density magnetic-recording devices, physicists are becoming increasingly more interested in the properties of magnetic materials on the nanometre scale. Current research efforts include the preparation of thin films and superlattices for improved data storage, the exploitation of electron spin rather than charge for device switching (“spintronics”), the development of new magnetic materials for biomedicine or drug delivery applications, etc.

In the evaluation of the Magnetic and Spintronic activities in the Condensed Matter Physics Groups in Sweden, we first look briefly at some of the issues involved in preparing new materials, characterising magnetic systems, and understanding the behaviour of these complex materials.

### Magnetic Research Activities

The understanding of the magnetism of matter is such that it appears unlikely that new bulk-type alloys and compounds with significantly improved intrinsic properties may be discovered. Tailoring the magnetic properties at the sub-micron or nanometre scale offers much more prospects, because the dimensions are below the characteristic length-scales of magnetic interactions or magnetic phenomena. Current research activities are therefore concentrated on magnetism in systems of reduced dimensions, where the distinction disappears between intrinsic properties, characteristic of a given magnetic phase, and extrinsic properties related to the detail of the microstructure. The main topics are: dynamics of nanostructured magnets, magnetic and magneto-transport properties of nanostructured wires and dots, microstructures and properties of nanocrystalline and nanogranular magnetic materials, hybrid organic–inorganic nanostructured magnets, etc. Recently, emphasis has been put on developing technologically relevant processes of low-dimensional structure production. If the structures are larger than about 10 nm, it is possible to use traditional “top-down” fabrication techniques, such as electron or ion beam lithography. In order to create atomically structured nanomagnets, researchers are instead trying to self-assemble the material from the “bottom-up”, using individual atoms.

The use of nanostructured ferromagnetic wires and films, allowing for switching in very small external fields, is of great interest for sensors, etc. Other research efforts are focused on the fabrication of confined systems with a lateral scale ranging from micrometers down to nanometres. Arrays of magnetic nanowires, synthesised by electrodeposition into nanoporous media, have also aroused a considerable interest. This templating method is very attractive, as it has proven to be reliable for the synthesis of arrays of nanowires and multi-layers of desired composition, microstructure, sizes, aspect ratios, and layer thickness. For magnetic nanowires, original

transport and magnetic properties have been identified, such as giant magnetoresistance, magnetisation reversal in a single nanowire, domain wall magnetoresistance, and other phenomena due to dimensions comparable to, or smaller than, scaling lengths in magnetism.

Among the various structures under investigation, one distinguishes also ferromagnetic spheres with nanometre diameter – and very promising for magnetic data storage at the high-density limit, e.g., the development of “quantum bits”, in which each bit of information is a unique magnetic subject. These nanomagnets, if embedded in an organic host, are also considered for applications in – biomedicine. For example, they can enhance the signal from Magnetic Resonance Imaging (MRI) using contrast agents made of magnetic nanoparticles that vary in size from 10 – 500 nm. Those particles-magnetic nanobeads can be injected into the bloodstream and, depending on their size, travel to different organs. Nanomagnets could also be used for drug-delivery. The magnetic nanobeads are first laced with drug molecules, and then steered by external magnetic-field gradients until they reach the desired parts of the human body. Approaches towards these applications include thin film deposition on structured substrates or the direct self-organisation of magnetic nanoparticles prepared by chemistry.

Although the patterns formed by fine-iron filings provide a crude visualisation of the magnetic field lines emanating from magnets, imaging complex magnetic structures on a finer scale requires a whole battery of more elaborate techniques. One of the most flexible techniques is the Magneto-Optical Kerr Effect (MOKE). Static and time-resolved MOKE can be used to study both magnetisation reversal and coherent magnetisation precession in exchange bias systems, e.g., ferromagnetic/antiferromagnetic layered structures. In static MOKE experiments, one uses separate longitudinal and transverse set-up geometries to simultaneously measure both longitudinal and transverse magnetisation components, respectively. Time-resolved MOKE enables one to study coherent magnetisation precession. Apart from other powerful magnetic imaging techniques, the focus is also on two particular techniques to investigate the magnetic domain configuration of micro-and nanomagnetic structures: Magnetic Force Microscopy (MFM) and Scanning Near-Field Optical Microscopy (SNOM). The MFM detects the magnetic stray fields, which are generated at the edges of magnetic elements (bits) or in domain walls. SNOM, contrary to any optical microscope, eliminates the need to distinguish diffraction patterns from one another and enables to overcome the diffraction limit.

In order to probe and tailor magnetic properties at the spatial limit, researchers have combined the Scanning Tunnelling Microscope (STM) with spin-sensitivity: Spin-Polarised Scanning Tunnelling Spectroscopy

(SPSTS). This is achieved by the use of ferro- and antiferro- magnetically coated probe tips, offering a high degree of spin-polarisation of the electronic states involved in the tunnelling process. Magnetic domain imaging with sub-nanometre-scale spatial resolution has been demonstrated for magnetic transition metal films. Ultra-sharp domain walls were discovered in ultra-thin iron films, while for ferromagnetic and anti-ferromagnetic samples, the different magnitude or orientation of magnetic moments could be made visible directly at the atomic level. The phenomenon of magnetic hysteresis has been observed at the nanometre length scale and has been correlated directly with microscopic processes of domain nucleation and domain wall motion. Magnetic switching phenomena of nanoscale magnetic islands and nanoparticles have been studied by time-dependent spin-sensitive STM imaging. Spin-sensitive STM measurements have also been applied to individual atoms and molecules on magnetic substrates. In particular, it has been shown that both the orbital symmetry, as well as the spin character of electronic scattering states around single atomic impurities, can be determined from real-space spin-sensitive STM data.

Another very interesting, but not often used, technique is SEMPA (Scanning Electron Microscopy with Polarisation Analysis), which enables one to excite secondary electrons from spin-polarised ferromagnetic surfaces. The advantage of SEMPA is its capability of measuring the magnetisation orientation, with a potential resolution below 100 nm.

It remains a challenge to elucidate how magnetisation reversal occurs in different types of patterned structures and complex systems like exchange biased materials. This mechanism can be studied using polarised neutron reflectivity techniques, which probe simultaneously magnetisation components parallel and perpendicular to the applied field. This vectorial magnetisation information allows discrimination between domain wall motion and rotation of the magnetisation. Finally, one of the most sensitive magnetic probes known is synchrotron based X-ray Magnetic Circular Dichroism (XMCD), which picks out tiny differences in the absorption of left and right circularly polarised X-rays. This effect can also be used to visualise magnetic domain structures. Switching from circular to linear polarisation, both ferromagnetic and antiferromagnetic materials can be imaged.

“Computer experiments” are also widely used to supplement experimental work in order to obtain a fundamental understanding of a phenomenon in terms of the physics. In particular, micromagnetic calculations allow a quantitative treatment of the interaction between magnetism and the microstructure of the ferromagnetic materials. They provide insight into the behaviour of new magnetic materials, optimally complementing or triggering detailed experimental studies. *Ab initio* computer simulations

have also developed rapidly, due to the continuous growth in computer power and improved numerical algorithms. They allow one to see what happens at the atomic level, such as the contribution of orbital and spin magnetic moment to the magnetisation at the interfaces between two materials, or to calculate the magnetic coupling of two magnetic layers across a non-magnetic region in a superlattice.

### Spintronic Research Activities

Other technologies will probably be required to address the so-called silicon roadblock some ten or so years from now, when silicon electronics reaches its limits. One such technology is based on controlling and manipulating the quantum mechanical spin of charge carriers, with which information will be encoded. We briefly review the emergent field of spintronics and describe some of the research possibilities. Major challenges in this field of spintronics that are addressed by theory and experiment include the optimisation of electron spin lifetimes, the detection of spin coherence in nanoscale structures, transport of spin-polarised carriers across relevant length scales and hetero-interfaces, and the manipulation of both electron and nuclear spins on sufficient fast time scales. It is envisaged that the merging of electronics, photonics, and magnetism will lead to new spin-based multi-functional devices, such as spin-FET (field effect transistor), spin-LED (light-emitting diode), spin RTD (resonant tunnelling device), etc.

The current research activities are still related to fundamental quantum aspects of spin phenomena in nanomagnetic structures. Formation of local spin and orbital magnetic moments, effective exchange interactions as well as different spin, charge and orbital ordering depends crucially on the electronic structures of real nanosystems. New theoretical approaches have been developed for an accurate description of the local quantum phenomena for correlated finite fermionic systems in a metallic environment.

The first step on the road of the use of the spin degree of freedom was the discovery of the Giant Magnetoresistance (GMR) of magnetic multi-layers in 1988. In specially designed multi-layers, known as spin valves, the magnetic configuration can be switched by a very small field inducing a large change of resistance. The first spintronic devices were based on spin valves, and today everybody has such a device on their desktops, since all modern computers use spin valves for the read heads of the hard disc. The magnetic tunnel junction (MTJ) is the second type of spintronic device that will soon have important applications for a new type of computer memory, the Magnetic Random Access Memory (MRAM). They are expected to reach similar densities and access times as the current DRAM or SRAM, but their main advantage over these volatile semiconductor-based memories

is that they retain data after the power is turned off, possibly eliminating the long boot-up time when the computer is switched on. Another important challenge is the search for ferromagnetic materials providing higher spin-polarisations than conventional metals, such as cobalt or iron. Interesting values of Tunnel Magnetoresistance (TMR) ratios have been observed in, e.g.,  $\text{La}_{2/3}\text{Sr}_{1/3}\text{MnO}_3$  (LSMO), but only at low temperature. Whereas the metallic spin devices provide new ways to store and read information in hard discs, tapes, or MRAM, semiconductor-based spintronics may offer a greater wealth of possibilities. First, they could combine storage, detection, logic, and communication capabilities on a single chip to produce a multi-functional device. The optical properties of the semiconductors are also of particular interest to transform magnetic information into an optical signal. Finally, manipulation of spins presents some advantages in terms of speed and required power over the manipulation of charge in conventional electronics. This has boosted research on diluted magnetic semiconductors (DMS), such as the archetypal GaAs doped with Mn, which displays ferromagnetic properties up to 150 K.

An important question is to what extent the manipulation of carrier concentration and spin-polarisation in semiconductor quantum structures can serve to tailor the magnitude and orientation of the magnetisation produced by spin localised on magnetic ions. Another issue is the elaboration of methods of injecting and transporting spin currents, which may lead to control over single spins in solid-state environment. The discovery of ferromagnetism in III-V compounds, such as (Ga, Mn)As, followed by the observation of ferromagnetism in p-type II-VI materials, such as (Zn, Mn)Te:N, allows one to explore the physics of the interesting combination of quantum structures and ferromagnetism in semiconductors. Extensive studies of ferromagnetic semiconductor heterostructures have led to the observation of a number of spin phenomena, such as spin injection as well as giant and tunnelling magnetoresistance. However, the practical applications of those systems in classical information systems have to be preceded by the synthesis of a functional material with a Curie temperature  $T_c$  above room temperature. Progress in this field requires development of growth and characterisation methods that enable better control over solubility limits, self-compensation, phase segregation, and precipitation of other compounds. To continue the rapid pace of discoveries, considerable advances are necessary in our basic understanding of spin interactions in the solid state, along with developments in materials science, lithography, and device fabrication. Progress toward understanding and implementing the spin degree of freedom in metallic multilayers and, more recently, in semiconductors is gaining momentum as more researchers begin to address the relevant challenges from different viewpoints.

## Magnetism and Spintronics in Sweden

The research efforts in magnetism and spintronics as part of Condensed Matter Physics in Sweden are described below. Two subsections focus on magnetic films and nanoparticles, and on semiconductors and spintronics.

### Magnetic Films and Nanoparticles

Work on magnetic films and heterostructures has its centre of gravity at Uppsala University, where an excellent consortium of the groups of Materials Physics, Solid State Physics /Magnetism and Theoretical Magnetism is formed. They also have collaborations with other universities in Sweden and with very well-known groups abroad.

The Materials Physics group of Björgvin Hjörvarsson has successfully carried out coherent and high-quality research by investigating and controlling i) quantum size effects in magnetic nanostructures and ii) the unique dimensional tailoring of magnetic heterostructures. This dimensional transition was accomplished by selective *in situ* doping by hydrogen, inducing a change from antiferromagnetic to ferromagnetic interlayer coupling. This reversible tuning of coupling in superlattices opens a new route to address the influence of exchange interactions. The group has not only the technological know-how to prepare high quality magnetic superlattices, but also possesses scientific creativity to perform original experiments and their detailed analysis. This work has enabled the group to establish a new set of findings, which are important for basic science, but also for such technological areas as magnetic data and hydrogen storage. As both domains are still at their exploratory stages, the continuation of these activities along the proposed plan is appropriate.

The magnetism activity at the division of Solid State Physics, headed by Per Nordblad, is concentrated on various topics in magnetism, e.g., spin systems, nanostructures and films, compounds as well as applications in the area of biotechnology. In the study of magnetic superlattices, the interest concerns mainly magnetic anisotropy and magnetoresistance properties. In nanomagnetism, arrays of sub-micron-sized magnetic structures are studied with emphasis on the magnetic structure and the nucleation process of domain walls. The results have been evaluated with a micro-magnetic simulator programme. In the area of biomagnetism, the group activities are centred on the use of externally operable sub-micron-sized magnetic elements in combination with colloidal magnetic nanoparticles. This group has cleverly selected key issues in the magnetism research area and has some major contributions in the field. The activities in the field of biomagnetism are innovative and should be pursued. The group applies interesting ways of analysing problems, with special attention to the

influence of surfaces and interfaces in magnetic nanostructures. Active collaborations both inside and outside Sweden should be encouraged and continued.

The theoretical efforts of Olle Eriksson's Theoretical Magnetism group involve magnetism of bulk materials, surfaces and multi-layers, molecular magnets, etc. Theoretical tools have been developed for calculating non-collinear magnetic properties, magnetocrystalline anisotropy, and magnetic phase transitions of solids. In the field of surface/thin film magnetism, they have used various methods to investigate spin and orbital magnetism, transport phenomena, etc. Although Eriksson's group started recently, he did not take long to establish himself as an expert in the area of surface magnetism. The work in the area of magnetic anisotropy energy is very impressive, and the future plans include extending the work to nanoscale magnets of various shapes and sizes. The goal is to understand the microscopic origin of the effect, and how it can be manipulated to produce technologically important materials with large magnetic anisotropies. Materials with unusual magnetic properties are in great demand, due to their possible application and the challenges that they provide to theoretical research. Olle Eriksson, Lars Norström and others have chosen to work in this very timely area, in which theoretical work is needed. Their outstanding work has a high degree of novelty and is likely to have large impact.

The very good research programme of Maj Hanson in the Solid State Physics group of Lars Walldén at CTH also covers a large number of topics. It is directed towards the development and fundamental study of nanometre size elements prepared from ferromagnetic films and magnetic heterostructures. Arrays of individual particles have been designed and are suitable for sensors and high-density information storage media. The static and dynamic magnetic properties of systems as a function of shape and size down to the nanoscale have been addressed through magnetisation measurements, imaging with MFM, as well as micromagnetic calculations. These activities resulted in a series of good quality publications during the last years. Hanson also collaborates with several groups, both Swedish (Uppsala) and international (Pittsburgh, Sony Corp.). An interesting recent development in this subgroup is to address spin-dependent transport and current-induced switching in confined systems using STM. This new direction is a valuable addition to the current experimental approach in the group.

As touched upon in the Surface Science section, the Surface Physics group of Nils Mårtensson at Uppsala University continues to play a major role in the study of composite nanostructured magnetic materials and characterisation of magnetic films and multi-layers. Examples are the

spin reorientation transition, which has been further clarified for ultra-thin multi-layering; the study of ordered arrays of magnetic nanoparticles and magnetic quantum dots; and the investigation of exchange bias in collaboration with EU partners.

Work on magnetic nanoparticles (see also the Nanoscience section) is performed at different locations in Sweden. It is worth mentioning the somewhat controversial pressure-induced ferromagnetism discovery in  $C_{60}$ , in which the Experimental Physics group (Tatiana Makarova) at Umeå University subsequently made several key contributions to this field. This group, headed by Bertil Sundqvist, has followed the tradition of high-pressure research at Umeå University, but carefully selected more topical subjects of fundamental interest. The accomplishments of Marakova, and the international interest in ferromagnetic fullerenes, prove the richness of this topical field as well as the quality of this excellent activity.

Collaborations between this group and Theoretical Physics group of Jörgen Rammer and Andrei Shelankov; also at Umeå University, are established with the main goal to identify the physical mechanism which drives the ferromagnetic transition in pure carbon compounds. They developed a theoretical model, using quantum chemical *ab initio* methods, which might allow the interpretation of the available experimental data. Jörgen Rammer is quite well known from a review article (1986) on the Schwinger-Keldysh technique for the study of transport phenomena. Recently, Rammer and Shelankov have broadened their very good activities, which is commendable.

Also within the domain of fullerenes and carbon nanotubes, an interesting low-energy implantation method has been used for the synthesis of magnetic-sensitive materials in dielectric matrices, where the ferromagnetic parameters depend on the metal/dielectric combination. Those studies, performed by the Atomic Physics group of Eleanor Campbell at CTH, demonstrate the great potential of using cluster beams instead of the more classical ion beams, and open excellent perspectives for the future activities in magnetism.

Within nanomagnetism, excellent activities are carried out by the Materials Chemistry group of Mamoun Muhammed, at KTH (see also the Nanoscience section). One long-term motivation for this group is to make a surfactant coating of magnetic particles for use as contrast agents in magnetic resonance imaging, and for targeted *in vivo* drug delivery. Further future activities in magnetism will include nanorods and nanowires with combined compositions, of interest for use in data storage and electronics. This kind of nanotechnology attracts a great deal of international attention. There is also considerable interest in low-dimensional magnetic systems, which exhibit strong quantum fluctuation effects and do not follow the usual semi-classical paradigms.

Mats Johnsson in Osamu Terasaki's group of Inorganic Chemistry (SU) is synthesising and characterising new low-dimensional antiferromagnetic spin compounds. The group is collaborating with theorists in Germany and Switzerland (C.Gros, W.Brenig, R.Valenti, and F.Mila) in studying their properties. Johnsson is playing an internationally recognised role in this field.

A young and impressive scientist within this area in Sweden is Carlo Canali at Kalmar University. The small theoretical group, headed by him, has chosen to work in the timely and intriguing area of nanomagnetism and spin-dependent transport in magnetic nanoparticles. Motivated by the experiments on magnetic SET's, he had already succeeded in the interpretation of the experimental results, using simple models for collective magnetisation and quasiparticle degrees of freedom. Quantum magnetisation in strong correlated systems and applications of the random matrix theory to disordered systems, are also subjects of his present work. Future work will focus on quantum magnetism and spin-dependent electronic transport, with the goal of understanding fundamental properties in the nanoscale region, as well as to engage in the important area of spintronics. The promising area of molecular magnets will also be examined. Despite Canali's somewhat isolated research environment at Kalmar University, he has managed to maintain a vigorous, successful, and excellent research programme.

Very good theoretical work within the nanomagnetism area is represented by Anna Delin's efforts, within the Applied Materials Physics group of Börje Johansson at KTH. She is applying first-principles techniques to understand magnetic properties of lower dimensional systems, particularly nanowires of 4d and 5d transition metals that are normally nonmagnetic. An interesting result is the prediction that nanowires of these metals should be magnetic, or more accurately super-paramagnetic, work that led to an invitation to write a review article in an international journal. Although the work of this group is application oriented, the work of Delin is fundamental and addresses topical phenomena in the field of nanomagnetism.

Finally, an exotic topic is the work on thin film organic-based magnets, performed by the group of Mats Fahlman (Organic Physics) at Norrköping Campus (and W. Salaneck at Linköping University). The research activities include fabrication, and study, of the materials properties of these systems, with the focus on room temperature ferrimagnets with semi-conducting properties. Besides the development of *in situ* physical vapour deposition (PVD), the properties of the thin film magnets will be determined mainly by synchrotron-based techniques. This very good research programme seems to have a very high potential. The group should also be aware of the danger of adding too many topics to their research efforts.

## Magnetic Semiconductors and Spintronics

There is a great deal of work within this area in Sweden, which is widely spread, both thematically and geographically. In the large constellation within Quantum Device Physics at CTH (Per Delsing), there is a subgroup (called “QuOx”), with Tord Claeson and Dag Winkler, which is focusing on spin devices, based on perovskite manganite ferromagnets, in order to produce magnetic tunnel junctions with Curie temperatures  $T_c > 300\text{K}$ . Grain boundaries, arranged in one- and two-dimensional arrays in thin films, are experimentally and theoretically studied as model systems. They recently observed magnetic order in 2D-arrays at temperatures 50 K above bulk  $T_c$ . Magnetisation reversal follows Stoner-Wohlfarth behaviour for single domain rotation when the magnetic field is applied perpendicular to grain boundaries. The long-term goal in the study of perovskite materials is the development of devices, which may be used in, e.g., radio astronomy, tele-communication, digital electronics, and medical applications. This excellent group uses state-of-the-art methods to produce thin film devices. The support provided by the clean room preparation facilities at Chalmers (MC2), and the available measurement systems (low temperature, high sensitivity) strengthen the possibilities of this subgroup and its ability to achieve the future goals.

At CTH, there is also very good work on electronic structure investigations of *in situ* MBE-grown III-V based semiconductors by Janusz Kanski in the Electronic Structure of Condensed Matter group of Per-Olof Nilsson, as mentioned in the Surface Science section. A recent development in this group are studies of (GaMn)As magnetic semiconductors, which are of interest for spintronics applications. These materials are metastable, and the capabilities of this group for *in situ* investigations are therefore valuable in terms of providing high quality experimental data for understanding the mechanisms stabilising the ferromagnetic phase. Of particular interest is the effort to develop growth conditions, which maximise the Curie temperature. The group has made significant contributions in this respect, which seem to be fully competitive and has triggered extensive collaborations with other Swedish groups, including laboratories at Uppsala and Lund, studying magnetic systems. Kanski is also actively participating in the development of the high-resolution beamline at MAX III, which will also provide opportunities for spin-resolved studies. The group has clearly shown the importance of *in situ* studies in their work, an advantage that should be maintained at MAX III.

The large Condensed Matter Theory group of Mats Jonson (CTH) has made an interesting theoretical proposal, which concerns spintronics: the possibility to manipulate the magnetisation of nanomagnets by electrical

means. In their scheme, the magnetic coupling is realised by a magnetic particle that is in contact with both nanomagnets via tunnel barriers.

Other excellent work is related to phenomena in which both electron coherence and nanoelectromechanical effects are important. They found that resonant tunnelling through a single-electron level might lead to giant magnetoresistance in spin-polarised nanostructures. The charge transport through single-electron transistor (SET) structures, the electromechanical instability in spin-polarised SET systems and the shuttle regime of spin-and-charge transfer will be studied. In the field of spin-flip processes in magnetic nanoconductors, the work has led to a new principle (and patent) for a compact solid-state laser in the 1–100 THz regime. The laser is based on a new mechanism, in which spin-flip processes in ferromagnetic conductors are created throughout the interaction of light with conduction electrons. The population inversion results from tunnelling injection of spin-polarised electrons from one ferromagnetic conductor to another. The work of this heterogeneous group of researchers is characterised by very innovative and creative projects, some of which must still be verified experimentally. Given the current trends in the field, the choice of the future research activities in the area of nanomagnetism, spintronics and related systems is timely and very appropriate. These excellent research activities in magnetism should be continued, preferably in close interaction with experimental groups.

In Uppsala, some groups of the strong consortium mentioned above are also highly active in this area. The Solid State Physics /Magnetism group of Per Nordblad is active in magnetic compounds and alloy systems. The current work focuses on 3d/4f compounds, single crystals of quasi-2D magnetic systems, as well as manganite and manganite-related compounds. The main interest is related to the study of exchange interactions, magnetic structure, magnetic anisotropy, and transition temperatures. An interesting aspect of these activities is the close co-operation with groups from Sweden (Uppsala), Vietnam, and India. They found a new compound with Beta-Mn structure and strongly frustrated bonds, and were one of the first groups to point out the close interplay between donor defects and magnetic properties in (Ga,Mn)As. Their future activities include magnetic semiconductor quantum wells and superlattice structures, two very topical areas with great fundamental interest and technological prospects. Another excellent activity by this group is the study of disordered and frustrated spins systems. This subject includes spin glasses, re-entrant magnets, diluted antiferromagnets, and magnetic nanoparticles. A common feature of these spin systems is that logarithmically slow dynamics develop at low temperature, and that the response function of any frustrated spin system is non-stationary and exhibits magnetic ageing. The present work is focused on fundamental questions

relating to the origin of this ageing phenomenon. Another unresolved question tackled by the group is the phase transition problem in 3D spin glasses and re-entrant systems. In particular, the question of a spin glass transition in a magnetic field remains controversial. In all the above-mentioned subjects, Nordblad's group has had a significant impact by performing careful measurements of magnetic dynamics and using these data for scaling analyses. They establish interesting contacts with a number of experimentalists and theoreticians in Japan and France.

The theoretical efforts of Olle Eriksson's Theoretical Magnetism group at Uppsala University involve general methods for solid-state physics, including magnetism of bulk materials, magnetoresistive effects, and structural and phase stability. They developed tools for calculating non-collinear magnetic properties, magnetocrystalline anisotropy, and magnetic phase transitions of solids. Combining first principle theory with Monte Carlo simulations, they proved the ability to calculate the critical temperature of any diluted semiconductor and investigated the influence of impurity concentration, lattice defects, and percolation phenomena in these materials. These studies contributed substantially to the key question in spintronics, as regard the materials properties. Materials such as diluted magnetic semiconductors are in great demand, due to their possible applications and because of the challenges that they provide to theoretical research. Eriksson and collaborators have chosen to work in this very timely area and are among the pioneers in the subject.

Olle Eriksson has his roots in the well-known Condensed Matter Theory (Uppsala) group of Börje Johansson, which is highly competitive and has made excellent contributions to, and applications of, density functional theory. The group has pioneered work in understanding and predicting structural stability, phase transitions, electronic and, in some cases, magnetic properties of advanced materials. In relation to the study of magnetic systems, the relatively young group member, Rajeev Ahuja (Ph.D. in 1991), has been involved in the development of a computational code for the magneto-optical Kerr effect (MOKE). Ahuja has an impressive publication list and is active in a large number of studies ranging from structural phase stability of materials to ceramics and Li-batteries. Another young group member, Susanne Mirbt (Ph.D. in 1995), studies the electronic structure of hybrid materials of ferromagnets and semiconductors. She has calculated the magnetic properties of substituted 3D-impurities in a GaAs host and explained their magnetic properties within a simple model. In the future, besides the search for high Curie temperature dilute magnetic semiconductors (DMS), she wants to relate the current understanding of the long-range ferromagnetic order in DMS to existing models. Susanne Mirbt

already has interesting scientific output in the field of magnetic properties.

Krister Karlsson at the University of Skövde is working in contact with Eriksson's group on *ab initio* studies of the temperature-dependent properties of magnetic materials. This is a challenging area, as popular applications of DFT are confined to very low temperatures. One of Karlsson's significant achievements is the proposed formalism for the calculation of the response function using a temperature-dependent Green's function. This has been used to calculate spectra and dispersion of spin-wave ferromagnets, such as Fe and Ni. Future work will involve calculations for magnetic semiconductors, in order to extract parameters for model Hamiltonia from first principles, for a variety of applications. This is a reasonable approach, especially in collaboration with O. Gunnarsson (Stuttgart) and F. Aryasetiawan (Lund/Tsukuba), who are leading experts in this field. This is also a smart strategy, since Karlsson's local environment may not be so ideal in a research field where there is great competition worldwide.

At KTH, the Nanostructure Physics group of David Haviland conducts excellent work on spin-dependant transport focused on the basic issues surrounding spin transport and

nanomagnetism: in particular, magnetic switching of very small nano-fabricated particles, in order to understand the energetic of the switching and to determine the thermal and quantum tunnelling limits for the magnetic particles to maintain their orientation (memory state). They also study spin injection in small magnetic particles via tunnel junctions and junctions formed at atomic interfaces. Adapting a fabrication technology to magnetic tunnel junctions, allowed them to study tunnel magnetoresistance (TMR) in new ways. The vision guiding these activities is to conceive and realise new device concepts for, e.g., the application of spintronics in areas such as memories and sensors. In particular, Magnetic Random Access Memory (MRAM) chips will in the future rely on a scaling to a very small size. The research activities of this relatively small group address a great variety of interesting and original ideas. They rely on expertise in nanofabrication, tunnel junction physics, and high frequency and scanning probe magnetic techniques on a nanoscale. The challenges are manifold, and the proposed research subjects are topical in this challenging field of magnetism. A valuable asset for future activities could be substantial theoretical support.

The Condensed Matter Theory group of Anders Rosengren at KTH studies the effects of disorder in quantum magnetism, such as the quantum Ising model, the quantum anisotropy XY spin chain in a random field, etc. Their work is based on numerical methods including Monte Carlo (MC) and Density Matrix Renormalisation Group (DMRG). A good method was found for exactly computing the partition function for the 2D Ising model

without an external field. In 3D, the approach was to use MC simulations with a newly developed method providing extremely detailed information. Overall, they are tackling a wide range of interesting theoretical problems ranging from random quantum spin chains to a 3D Ising model. This is an excellent theory group with a number of important papers, a healthy balance of interesting research projects, and a good group dynamic, which encourages both collaboration and independence.

The Condensed Matter Physics group at Campus Kista of KTH consists of two very good subgroups, one led by Alexander Grishin and the other by Magnus Andersson and Östen Rapp (see Superconductivity section). The first subgroup carried out extensive studies on crystal growth and device applications of various oxides-related functional materials. For example, Grishin showed that thin film Mn oxides, which are widely studied for their colossal magnetoresistance (CMR) effect, also have potential as an excellent material for non-cooled IR bolometric devices. More fundamentally, it was shown that in manganites the exchange interaction responsible for CMR is suppressed by electron confinement. A novel approach used by the group is to combine non-compatible properties in a single oxide-based heterostructure. For example, the group has succeeded in growing heterostructure multi-layers, which can combine colossal magnetoresistors with piëzo- and ferroelectricity. Although each of the research subjects is well chosen and has resulted in quite interesting results, one cannot avoid an impression that the efforts of this subgroup – taking also into account the non-magnetic activities – are too widely distributed.

The main activity in magnetism of Ulf Ekenberg (Photonics and Microwave Engineering at KTH, Campus Kista) aims to process information using the spin degree of freedom of the electrons. The spin-FET has not yet been realised due to difficulties in the injection of spin-polarised currents from metallic ferromagnets to semiconductors. A possible way to overcome the obstacles is to use magnetic semiconductors, such as MnGaAs (p-doped), as contacts for the Spin-FET. Ekenberg's emphasis is on the calculation and simulation of various spin-tube transistor configurations. In particular, he has been studying band splitting due to spin-orbit coupling, associated with the Rashba effect. This area is potentially important for the proposed Data-Das spin transistor. Together with his post-doc Dejan Gvozdic, he has studied a fairly realistic model for several III-V semiconductors, which includes conduction, heavy hole, light hole, and split-off bands. They tentatively concluded that the Rashba effect is much larger for holes than for electrons. Ekenberg's good work anticipates that an experimental group that he is associated with at KTH will test these interesting theoretical predictions.

The Materials Science group headed by Bo Monemar in Linköping (see also the Semiconductor section) has carried out an extensive research programme on compound semiconductors and devices with, e.g., emphasis on magnetic semiconductors, such as  $(\text{CdMnZn})\text{Se}$ ,  $\text{GaMnN}$ , and  $\text{SiMnC}$ , which may well play key roles in the spintronic area. In co-operation with the Ioffe Institute (Russia) and the University of Florida, they develop suitable dilute magnetic semiconductors such as  $\text{GaNnN}/\text{InGaN}$  for a spin-LED that is ferromagnetic at room temperature. The research work on magnetic semiconductors by this group is unique, in that Mn atoms are incorporated into a set of wide-gap materials, e.g.,  $\text{SiC}$ ,  $\text{GaN}$ , and  $(\text{CdZn})\text{Se}$ . In fact, theorists have predicted that the Curie temperatures can be substantially increased in  $\text{GaMnN}$  and other wide gap materials. This is an excellent and highly qualified group of semiconductor materials researchers. The senior researchers are very experienced and well recognised internationally. The group has a substantial infrastructure for sample growth and characterisation. Careful future work by this group in magnetic semiconductors will be highly valued.

Igor Zozoulenko, of the Mesoscopic Physics and Nanoelectronics group, recently moved from Linköping to Norrköping and works mainly on trajectories and wave functions of non-interacting electrons in confined structures, such as quantum dots, multi-quantum dots, etc. His future plans are also related to spintronics and quantum transport in quantum dots, exploring the possibility to use them as controllable spin injectors, spin filters and spin detectors. He has apparently continued collaboration with different experimentalists and seems to have carved a niche for himself, doing fairly elementary calculations involving non-interacting electrons in various geometries.

In Lund, there is an interesting activity in spin phenomena on the theoretical side. For instance, the excellent research of Stephanie Reimann in Sven Åberg's group of Mathematical Physics is focused on electronic and spin structures of dot lattices. She has found a systematic magnetic behaviour of square quantum dot lattices. Other interesting work was related to broken spin symmetries in quantum dots, both within the spin density functional approach and exact diagonalisation studies. She has an ongoing collaboration with groups in Finland, Denmark, and Germany, and she has obtained a number of interesting results on the ground state of finite systems. Reimann is involved in topical research projects, bringing in fresh ideas and combining different theoretical approaches, which merits encouragement.

Theoretical activities are also carried out in the Solid State Theory group at Lund University. Carl-Olof Almbladh and Ulf von Barth are many-body theorists, well known for their work in self-consistent calculations. In the

last few years, they have done much fundamental research work on the dynamical properties of polarised spin systems, especially in semiconductor heterostructures. It was recently predicted that in a narrow gap III-V semiconductor quantum well an electron spin current can be generated, which can modify the Rashba spin-orbit coupling constant. Almladh and von Barth are interested in bringing fundamental changes into computational methodology, in order to address some challenging issues. The Expert Panel has the impression that both have made quite important contributions to fundamental issues in density functional theory. On the other hand, they may have been doing rather similar things for a long time, and in a slightly less innovative way as before.

In Lund, it is also worth noting the activity by the Synchrotron Radiation Research group of Jesper Andersen, discussed in the Surface Science section, which has recently been developing means to cleave *in situ* III-V semiconductor compounds (XSTM technique), making it possible to obtain atomically resolved STM images of, for example, ferromagnetic semiconductor compounds and superlattices. While in principle this methodology is well established by others, this is not routine in character, and the information gained gives new and important insights into these materials.

## Future Perspectives

The theoretical advances and the strong involvement of magnetism in all branches of technological development make this discipline one of the most relevant areas of current research in Condensed Matter Physics. The capabilities for materials fabrication with control at the nanoscopic level, and the development of new instruments, are the basis of emerging and interdisciplinary activities in magnetism. Since magnetism activities are carried out at many research institutes all over the world, only a well-orchestrated and concentrated effort will guarantee success in the future.

Despite the many possible applications of nanomagnets in biomedicine, the field is still driven by the search for faster, cheaper, and higher-density magnetic-storage devices and sensors. The three main challenges are to design new types of magnetic nanostructures, to control the way in which spin-polarised electrons move in such materials, and to ensure that such structures can be made cheaply in large quantities. To continue the rapid pace of discoveries, considerable advances in our basic understanding of spin interactions in solids along with developments in materials science, lithography, and device fabrication are necessary. Progress toward understanding and implementing the spin degree of freedom in metallic multi-layers and, more recently, in semiconductors is gaining momentum.

With contributions from a diversity of fields including physics, chemistry, biology, electrical engineering, computer science, and mathematical information theory, the rapidly emerging field of spintronics promises to provide fundamentally new advances in both basic and applied science.

Although it is always problematic to try to predict the future, a few issues within the magnetism and spintronic field in Sweden can be addressed. The research activities appear very healthy with more than 25 CMP groups active, and many participating in internationally recognised networks. The current topical areas seem to be well covered, including magnetic thin films, heterostructures, nanoparticles, magnetic semiconductor perovskites, and many aspects of spintronics.

Concerning the experimental characterisation possibilities available to the Swedish magnetism community, it might be of interest to implement two very interesting measuring set-ups: time-resolved magnetic PEEM (TR-XMCD and TR-XMLD), which is one of the most exciting prospects in the field of magnetisation dynamics, and available in some synchrotron radiation laboratories; and spin-polarised scanning tunnelling spectroscopy (SPSTS), which combines scanning tunnelling microscopy with spin sensitivity.

Within the area of magnetic semiconductors and spintronics, a stronger collaboration of the CMP laboratories in Sweden, or some kind of unified approach, is commendable. The strong interest and fast progress, in this topical field, of the research activities in many applied-oriented laboratories, as well as in industry, should be taken into account in defining future activities.

Overall, the future for magnetism and spintronics in the Condensed Matter Physics Community in Sweden is very promising and seems ready to compete with some of the best groups on an international level.

## Semiconductors

### International Perspective

Over the last fifty years, research activities on semiconductors have played extremely important roles both in condensed matter physics and in electronics. Indeed, extensive investigations of Si, Ge, GaAs, AlGaAs, and related materials and structures have resulted in a number of significant discoveries and inventions. They include the advent of bipolar transistors (1947 – 1948), MOS-FET's/HEMT's ('60,'80), LSIs ('58), tunnel diodes ('58), diode lasers ('62,'70), CCDs ('70), and integer/fractional quantum Hall effects ('80,'82). They have greatly expanded the forefront of science and also laid the solid foundation for advanced technology.

In addition, numerous exploratory works have been performed on the growth and patterning of semiconductors in order to form various nanostructures, such as quantum wells (QW's), superlattices, quantum wires (QWR's), nanotubes, and quantum dots (QD's); indeed, electrons confined in such low-dimensional systems have been found to exhibit unique and attractive properties, as well as new and useful device functions.

Semiconductor research is quite diverse and covers a wide range of subjects. One way to represent a specific research subject is to define a point  $(x, y, z)$  in a three-dimensional (3D) space, where "x" represents the constituent elements of a semiconductor, "y" its structure, and "z" its properties or functions. For example, one-dimensional electron transport in carbon nanotubes, single photon generation from a single InAs QD in GaAs matrix, growth chemistry of GaInN/GaN QW's, and ferromagnetic properties of ZnMnO films are representative topics, which reflect broad spectra of semiconductor studies.

### Diversity of Semiconductor Materials

For the sake of convenience, we begin by presenting a perspective of the field by viewing numerous research subjects on the basis of semiconductor materials; they range from elemental semiconductors, such as Si, Ge, and C, to various compounds, including GaN, ZnO, and TiO<sub>2</sub>. These semiconductors can also be classified into three categories, depending on their stages of development.

In the case of classic materials, such as Si, Ge, GaAs, InGaAs, and related compounds, most of their bulk properties and functions are pretty much understood, and their new aspects and associated potential are now explored, mostly after they are shaped into various device structures and/or nanostructures, as will be discussed later.

GaN, SiC, ZnO, and related compounds are also well-known classic materials, but can be categorised as materials of delayed take off. This is because their qualities and controllability have been drastically improved in recent years, from an unsatisfactory level, to a quite dependable one. Consequently, their attractive properties and device potential have been extensively disclosed only recently, giving birth to blue-light emitting diodes and new high-voltage power devices, as will be elaborated later.

In the case of GaN and other nitrides, it was demonstrated by Japanese researchers that the quality of epitaxial films can be improved dramatically by inserting an AlN (GaN) buffer layer, grown on a lattice mismatched sapphire substrate at low temperatures. Currently, the possible use of alternative substrates, such as SiC and GaN, has been investigated. In addition, p-type doping of GaN layers, which had long been tried in vain, was finally

made possible by introducing a post-growth annealing process, in which hydrogen atoms, responsible for the inactivation of dopants, are driven out of the doped layers. These breakthroughs have opened a new and exciting research field, where physics and electronics applications of nitrides are explored. Similarly, p-type doping of ZnO layers was finally achieved quite recently, allowing the fabrication of ZnO-based new photonic devices, such as blue LED's.

Advances in epitaxial growth technology have given births to a set of new semiconductor materials. One such example is a class of diluted magnetic semiconductors (DMSs), such as GaMnAs and InMnAs, which are synthesised in recent years by introducing Mn atoms into III-V compounds. They have attracted strong interest, since their magnetic properties are dependent on their hole concentration and, hence, may well be controlled by electrical or optical means. Though their Curie temperatures  $T_c$  are well below 300K, attempts are made to raise  $T_c$ , especially by introducing Mn atoms into wider gap materials, such as GaN, and SiC. More familiar II-VI based DMSs, such as CdMnTe, have been actively studied, and their magneto-optical properties and functions intensively explored.

Another example of newly developed semiconductors are diluted nitrides, such as GaNAs and GaInNAs, where the introduction of a small amount of nitrogen atoms, one or a few percent in content, gives rise to a substantial decrease of the band-gap in host materials. This anomalous and yet important behaviour is ascribed to the interaction of the GaAs conduction band, with unique electronic states that are localised around single or multiple nitrogen atoms. Their use for lasers in optical communication systems and for novel tandem solar cells is intensively investigated.

Finally, a brief statement should be made on a family of new oxides, in which correlated electrons play important roles. Although many of these materials have been studied with the main focus on their high- $T_c$  superconductivity, some of them exhibit unique transport properties that depend sensitively on temperatures and magnetic fields. Both the mechanisms and possible applications of these phenomena are intensively investigated.

## Nanostructured Semiconductors and Surfaces

### *Layered Nanostructures and Surfaces*

Semiconductor surfaces and interfaces exhibit a variety of properties, which are quite different from those of bulk semiconductors. Since surface physics studies are described in another section of this report, we here describe only nanostructures surrounded by interfaces and/or surfaces.

For the last 15 years, major conferences and journals on the physics of semiconductors have been dominated by papers on nanostructured

semiconductors and low-dimensional electrons confined therein. In fact, studies of the physics of two-dimensional (2D) electron systems in nm-scale channels of Si MOS FET's began already in the middle of the 1960's. This field of 2D electron physics experienced an explosive expansion in the 70's and 80's, mainly due to two factors; the discoveries of integer and fractional quantum Hall effects (QHEs), and the advent of epitaxially grown GaAs/AlGaAs quantum wells (QW's), superlattices (SLs), selectively doped high-mobility heterojunction channels, and other layered nanostructures.

The discovery of QHEs has expanded the field by disclosing the rich physics of magnetically quantised 2D-electron systems; they include features of the quasi-ballistic transport through edge channels and the fascinating behaviour of electrons, originating from their many-body interactions. On the other hand, the advent of GaAs/AlGaAs, QW's, SLs, and related heterostructures has immensely enriched the field of 2D-physics by providing extremely high mobility electron systems needed for high-speed transistors and mesoscopic transport studies. These heterostructures have also enabled basic physics studies and device applications of electron tunnelling phenomena normal to the layers, as well as optical transition processes between the conduction and valence bands. Indeed, the majority of lasers, LED's, and other interband photonic devices, widely used today, utilise quantum well (QW) layers in their core parts. Moreover, several new mid-infrared (MIR) and terahertz (THz) devices, such as quantum cascade lasers and quantum well infrared detectors, have emerged by making clever use of both inter-subband optical transitions and cross-barrier transport of electrons in these heterostructures.

### *Quantum Dots, Quantum Wires, and Related Structures*

In the mid '70s and the early '80s, a couple of theoretical papers appeared, in which the control of electrons by quantum wire (QWR) and quantum dot (QD) structures was proposed, and the possible uses of one-dimensional (1D) and zero-dimensional (0D) electrons for novel transport devices, FET's, lasers, and non-linear optical devices were discussed. In the mid '80s, electron beam lithography and patterning techniques were successfully applied to fabricate prototype QWR's, QD's, and related nanostructures with typical sizes of 100 nm. Since then, quite a lot of pioneering work on 1D and 0D electrons structures has been accomplished; this includes the quantisation of conductance resulting from the ballistic electron transport through short QWR's (i.e., quantum point contacts), Aharonov-Bohm oscillations in the magnetoconductance of ring-shaped samples, and many other consequences of quantum interference in QWR's. As for lithographically defined QD systems, various unique properties, such

as single electron transistor (SET) actions, shell structures of discrete levels, billiard-like trajectories, the Kondo effect, and so on, have been disclosed.

For most of the device applications, QWR and QD structures of 10 nm or less in size are strongly desired, as the energy level spacing must be large enough to accommodate electrons mostly in the ground state. To make such structures, a variety of growth methods has been developed, as later described more in detail. For example, 10 nm-scale GaAs and InGaAs wire structures have been successfully fabricated in the bottom part of grooves, or on the top part of ridges, which were formed by selective facet growth on patterned substrates. The overgrowth of a quantum well or an n-AlGaAs layer on the cleaved edge of pre-grown GaAs/AlGaAs quantum well structures has also been used to form 10 nm-scale QWR states. Unique features of 1D electrons and excitons in these structures, such as the enhanced binding energy of 1D excitons, have been disclosed. Moreover, these QWR structures have been incorporated into the core parts of FET's and lasers, and their unique device performance has been demonstrated.

About ten years ago, a researcher at Hitachi reported that 10 nm scale pillar-shaped InAs QWR structures can be grown on selected spots on a substrate by depositing tiny Au particles beforehand. In recent years, this method has been intensively studied and developed at Lund University and at Harvard, where a variety of QWR's are synthesised and their new properties and functions disclosed. As this approach allows the wire composition  $n(x)$  and the electronic potential  $V(x)$  to be modulated along the wire axis, it has been successfully used to form quantum dots, SET's, pn junctions, and other 1D structures.

Similarly, it has been found that carbon nanotubes (CNT's) of various sizes and chiralities can be spontaneously grown at selected spots on a substrate where tiny Fe islands are pre-deposited. Semiconducting CNT's formed in this way have been widely investigated to disclose their new properties and functions, including novel luminescence phenomena from strongly bound 1D excitons in CNT's, and the gate voltage controlled transport of 1D holes and electrons in CNT FET's.

For self-organised growth of nm-scale quantum dot structures, several methods have been developed. For example, selective growth near the apex of a pyramidal structure, or near the bottom of an inverse pyramidal recess, is used to form a single dot with well-controlled shape and location. The spontaneous formation (due to Stranski-Krastanov growth) of dense and tiny semiconductor particles on lattice mismatched substrates has been employed to fabricate 10 nm scale QD's of various compositions. InAs QD's on a GaAs substrate, in particular, have been intensively studied to clarify their quantum level structures, photonic, and transport properties, and

novel device functions. For example, these dots are now implemented in the core parts of QD-based lasers, detectors, memories, and single-electron transistors. Moreover, colloidal processes to form nm scale semiconductor dots in liquid or vapour phases have been developed to fabricate isolated QD's of various shapes and compositions. Their photonic properties, including size-dependent luminescence spectra, have been clarified, and their uses as bio-medical fluorescent markers demonstrated.

### *Device Applications and Their Socio-Technological Impacts*

Since the birth of bipolar transistors in 1948, research activities on semiconductors have been conducted in a unique environment, in which two-way interactions between basic physics research and applied device research have stimulated and enriched both parties. For example, studies on Ge bipolar transistors and Si MOS field effect transistors (FET's) have not only led to the amazing progress of computers, but also induced the invention of tunnel diodes by L. Esaki and the discovery of the quantum Hall effect by K. von Klitzing, respectively.

In addition, exploratory studies on III-V compounds have not only had a huge impact on photonics and fibre/wireless communications, by giving birth to heterostructure lasers and high-speed transistors, but have also induced the discovery of fractional quantum Hall effect by D. Tsui and H. Stormer, as amazing developments of quantum well physics and electronics. Another notable contribution of semiconductor research to information technology (IT) is the advance of flat panel displays, where InGaN blue LED's, organic LED's, and/or amorphous Si thin film switching transistors play critical roles.

To expand the forefront of IT, a couple of extreme devices have been developed that utilise only one electron. The single-electron transistor with ultra-high charge sensitivity is a representative example. Single-photon emitters/detectors are another example and have recently been achieved, mainly to realise quantum cryptographic systems. Moreover, semiconductor qubits that are based on either electron charge or spin, or nuclear spins, have been explored to lay foundations for the possible realisation of quantum computers.

The societal impact of semiconductors is not restricted to the realm of IT, but is now extended to cover such important fields as energy/ecology and bio/medical technology. For example, a variety of semiconductor materials are now intensively studied to make more efficient solar cells, thermoelectric devices, GaN-based solid-state lighting devices, high-voltage power controlling devices, etc. Various sensor systems are being developed using new semiconductor structures. Quantum cascade lasers and quantum well

infrared detectors (QWIP's) have provided unique gas sensing and thermal imaging capabilities, covering the spectral range from the mid-infrared into part of the THz regime. Chemical sensor applications of semiconductors, such as granular films and carbon nanotubes, are also being explored, since chemisorbed gas species influence their electrical conductivities. The use of quantum dots as fluorescent biomedical markers and labels has been almost established, and some of their advantages over fluorescent dyes are clarified. Photocatalytic functions of  $\text{TiO}_2$  are now widely used, since bacteria and other organic contaminants are decomposed by oxygen atoms generated by the photochemical dissociation of water on  $\text{TiO}_2$  surface.

### *Micro- and Nanofabrication Methods and Their Role in Science*

A variety of methods has been developed to form various semiconductor structures and devices. They can be categorised into two groups: one for the preparation of layered structures and the other for the in-plane patterning of semiconductor structures and devices. It should be noted that these fabrication methods are indispensable, not only for semiconductor electronics and for physics, but also for other branches of condensed matter physics, such as magnetic and superconducting materials.

As pointed out elsewhere, molecular beam epitaxy (MBE), metal organic chemical vapour deposition (MOCVD), multi-target sputtering, and other film growth methods, have been developed to prepare a number of layered semiconductor heterostructures, in which the thickness, composition, and purity of constituent layers are controlled with extremely high precision. They are now widely used to form quantum wells, selectively-doped heterojunctions, superlattices, and single/multiple barrier tunnelling structures, where quantum confinements and/or tunnelling of electrons play decisive roles. As a result, new areas of semiconductor physics and electronics have been opened, where attractive properties and functions of 2D electrons and excitons are studied and exploited. Here, one should note that these methods have now been extended to other fields of science, including magnetism, superconductivity, and X-ray optics, where the multi-layered nanostructures offer very important possibilities.

Another important area of semiconductor technology is advanced lithography and other processing methods used for the 2D or 3D patterning of semiconductors. For instance, advanced lithographic methods, which have been developed mainly to fabricate Si LSI and other semiconductor devices, are now widely used to pattern a variety of other materials and devices. Indeed, the lithographic patterning of metals, superconductors, and magnetic and photonic materials now play extremely important roles at the forefront of the respective research fields. It is noteworthy that novel nanoscale

patterning methods other than the standard electron beam lithography have been developed; representative examples are the nanoscale manipulation of atoms and nanostructures with an STM tip, local anodic oxidation by a conductive AFM tip, and imprint lithography for organic materials.

In addition to the lithographic methods, several unique growth techniques have been developed to form various semiconductor nanostructures, as described above. For example, self-organised growth techniques developed mainly for semiconductor nanoparticles and nanowires may well play important roles in other fields, since they are often applicable to other materials systems.

### *Theoretical Activities*

The forefront topics of semiconductor physics have been explored by collaborative interactions of experimentalists and theorists. In some case, an unexpected discovery, such as the fractional quantum Hall effect, is followed by related experiments and theoretical studies, which disclose the mechanisms, other facets, and the essence of the phenomenon. In other cases, new concepts, or phenomena, such as the Bloch oscillation in superlattices, are first proposed or predicted and later proven or disproved by experimental studies. Thanks to the great progress of computers and related codes, computational physics studies are extensively conducted in recent years to clarify the electronic structure of various materials systems and also to predict their properties. Since theoretical work is discussed in another section of this report, we here point out only a few topics relevant to semiconductors.

Features of eigenstates of quasi-zero dimensional electrons and excitons confined in quantum dots (QD's) of various geometries and materials have been theoretically studied to clarify such unique aspects as their shell structures, exchange and correlation effects, interactions with other electrons in neighbouring dots and electrodes, including the Kondo effect, in the presence and/or the absence of magnetic fields. In addition, electron transport phenomena via localised states in various QD and organic molecular systems, as well as intra-dot relaxation and de-coherence phenomena of electrons, including their spin and polaron effects, have also been investigated theoretically. The unique behaviour of quasi one-dimensional (1D) electrons and excitons confined in various QWR and carbon nanotube (CNT) structures have been theoretically studied; they include size and chirality-dependent band structures of CNT's, huge excitonic effects in CNT's and QWR's and their roles in optical spectra, and Luttinger-Tomonaga liquid behaviour of interacting 1D electrons in QWR's. The origin of a novel "0.7 conductance anomaly" (see "Quantum wires..." section below) in the quantised conduc-

tance characteristics of quasiballistic QWR's are theoretically discussed in connections with the spin polarisation. A number of theoretical studies are being pursued of unique electronic states that can be generated in single and double layer quantum Hall systems (QHS) under various filling conditions, including the composite Fermion states in the vicinity of half-filled Landau levels. The current-induced polarisation of nuclear spins of Ga and As atoms in QHS is also being analysed in connection with its possible use for quantum computation. In relation to spin physics in semiconductor and spintronics, extensive theoretical work is being conducted on such subjects as carrier-mediated ferromagnetism in GaMnAs and related materials, the control of the Rashba effect for spin transistors, and the control of spin states in single and coupled QD systems for qubit applications. For other important theoretical activities, see the Condensed Matter Theory section.

## Semiconductor Studies in Sweden

### *Si, SiGe, SiC, C, and Related Materials*

Si-based electronics, such as LSIs, CCDs, solar cells, and power-controlling devices have continued their evolutionary but amazing growth over the last several decades, mainly by miniaturisation of device structures, and partly by exploratory utilisation of new materials other than Si. For example, the efforts of Shi-Li Zhang (Materials and Semiconductor Physics, KTH) to make use of SOI (silicon on insulator) wafers for high-frequency Si transistors and MEMs are technologically relevant and have laid the basis to form novel Si nanowire structures. The miniaturisation technology, especially nanoscale lithography developed in this field, has created important openings not only in advanced Si electronics, but also to the field of nanoscience and technology, as described in subsections "Quantum wires..." and "Quantum dots ..." below. Hence, efforts at KTH, MC2 (Chalmers), Uppsala University, and other locations to establish and utilise micro- and nanoprocessing capabilities for basic research can be positively evaluated. Of course, one needs to pay attention to the cost effectiveness of these facilities and establish sustainable systems, as the running cost tends to be rather high.

As for SiGe alloys, researchers both at Linköping University (Wei Xin Ni and Göran Hansson) and at KTH (Shi-Li Zhang) have played leading roles and made very good/excellent contributions in establishing the epitaxial growth of Si-Ge-based heterostructures and their device applications. Although these systems have been quite well studied and are now used in commercially available high-speed transistors, exploratory efforts to develop the full potential of SiGe are quite appropriate. One such example is the work on SiGe MOSFET's by Zhang (KTH). Moreover,

exploratory research of Uhrberg, Hansson, and Ni to exploit Si-Ge-based nanostructures for quantum cascade lasers, quantum dot phototransistors, and Er-doped HBT's can be positively evaluated.

Research activities on SiC pursued both at Linköping University (Bo Monemar's group) and at KTH (Margareta Linnarson and Nils Nordell *et al.*) in collaboration have played a leading role in the recent development of this noteworthy field. The hot-wall chemical vapour deposition (CVD) method developed in Linköping (in collaboration with Epigress Co.) and VPE growth on non-planar substrates (Nils Nordell, KTH) are important steps for the growth of high-quality SiC, in which point defects, dislocations and polymorphisms need to be suppressed and dopant incorporation controlled. SiC is a promising wide gap material, particularly for the next-generation high-voltage power devices. Hence, studies on the interface properties of SiO<sub>2</sub>-SiC MOS systems and metal-SiC Schottky barriers, performed by Leif Johansson *et al.* (Materials Science, LiU), and doping studies conducted both by E. Janzén *et al.* (Materials Science, LiU) and by M. Linnarsson (KTH), are quite important as they determine the performance of power devices. Similarly, studies of atomic diffusion in SiC (at KTH by Linnarson *et al.*) are also important and to be continued. SiC power devices are expected to gradually replace some Si power devices, even though views of industrial specialists are somewhat divided on the pace at which this transition will take place. An effort at LiU to prepare high-quality SiC substrates for GaN-based devices is also technologically quite significant. A novel effort to grow ferromagnetic SiCMn will be described in another subsection ("The II-VIs,...") of this report. SiC related research activities both at Linköping University (LiU) and at KTH are partly excellent, partly very good.

As for different forms of carbon, not much work is done on diamond, but research activities on semiconducting carbon nanotubes are quite actively pursued in Sweden, as mentioned in another part of this report.

### *The III-V Compounds, Such as GaN, AlGaIn, GaInN, and GaInNAs*

The III-V compound semiconductors play an extremely important role in both physics and device applications. For many of these, such as GaAs, InGaAs, and InP, bulk properties have been so well studied that their new aspects are now mainly being investigated after they are shaped into various devices or nanostructures, as will be discussed further on.

For GaN, (AlGaIn)N and related nitrides, however, the situation is different, as many of their new possibilities and problems have been disclosed only in the last ten years. Although rapid developments in this field have already resulted in the commercial production of blue light-emitting diodes and lasers, numerous potentials and problems remain to

be studied or solved. For example, the extension of the spectral range of nitride-based light emitters from the ultraviolet (UV) all the way to the infrared (IR) region, and also the establishment of GaN-based transistor technology for high-power/high-speed applications, are very important not only for advanced IT systems, but also for energy saving lighting and sanitation systems.

The research group of Bo Monemar (Materials Science, LiU) and collaborators has played a leading role in this rapidly growing field and has made a series of outstanding contributions to materials science and device physics of nitrides. In particular, both technology and materials science aspects of epitaxial growth processes, such as hot wall MOCVD and VPE, have been extensively studied. This research covers not only the growth of GaN, AlN, their alloys, and their heterostructures on various substrates, but also more exploratory nitrides, such as InGaN and GaInNAs, where InN clusters and N-based localised states are considered to play important roles, respectively. Studies of the mechanisms of bandgap reduction and annealing effects in GaNAs, made by Irina Buyanova and Weimin Chen (Materials Science, LiU) – and those of the unique behaviour of excitons and acceptors in these nitrides – are quite important, not only for nitride-based devices (lasers, LED's, and detectors), but also for the basic understanding of electronic and photonic properties of nitrides, where strains, piezoelectric fields, polarities, and localised states play significant roles. Note also that the accumulated experience of these nitrides is now employed in the field of spintronics by growing GaMnN and related magnetic systems.

A couple of other groups in Sweden investigate the growth of GaN and related nitrides by employing alternative methods, such as MBE (Thorvald Andersson, Microwave Electronics, CTH) and PVD (Lars Hultman, Thin Film Physics, LiU). They have provided complementary insights into these important materials systems, as described in subsection "Theoretical works...". Note also that Nordell's group (Materials and Semiconductor Physics, KTH) explores the use of GaN/AlGaIn heterostructures for high-speed transistors (HEMT's), LED's, and inter-subband transition (ISBT) photonic devices, which is quite appropriate, as stated more in later paragraphs.

### ***The II-VI, Oxide and Magnetic Semiconductor, and related materials***

Compound semiconductors, containing group II and/or group VI elements, have been studied for a long time, but their role in physics and electronics has been far smaller than that of III-V compounds. Recently, however, they have started to attract renewed attentions; for several reasons mentioned in the previous section. Among them, GaMnAs, SiCMn, and other Mn-doped dilute magnetic semiconductors (DMS) have gained intense interests,

as their carrier-induced ferromagnetism may well be important, for both physics and spintronic applications. Electron-spectroscopic (MAX) studies of Mn diffusion in GaMnAs, investigated by Janusz Kanski (Electronic Structure of Condensed Matter, CTH/GU), and annealing studies of donor defects in GaMnAs, by Peter Svedlindh/Per Nordblad's group (Solid State Physics, UU), have provided unique insights into the structure – property relationships of this interesting system. Theoretical work by the group of Olle Eriksson (Theoretical Magnetism, UU) provided new insights into GaMnAs, including the important roles of defects and percolation in this system. Work at Linköping University (Materials Science) to synthesise and investigate GaMnN, SiCMn, ZnMnO, (CdZnMn)Se, and other wide gap DMS (Irina Buyanova, Weimin Chen, *et al.*) are valuable attempts, as their Curie temperatures are expected to be much higher than that of GaMnAs.

ZnO, TiO<sub>2</sub>, and other semiconducting oxides and chalcogenides have also attracted strong renewed interest, since their qualities are drastically improved by advanced growth techniques. As a result, their interesting properties and important functionalities are now being disclosed. For example, unique insights have been obtained into the photocatalytic action of nanostructured TiO<sub>2</sub>, at Uppsala University (UU), by photoelectron spectroscopy (the group of Hans Siegbahn and Håkan Rensmo, Electron Spectroscopy and Molecular Surface Physics). Börje Johansson's group (Condensed Matter Theory, UU) has theoretically shown the possibility of a superhard crystalline phase of TiO<sub>2</sub>. The group of Claes-Göran Granqvist (Solid State Physics, UU) has conducted extensive studies of various oxides, with the main aim of using them as electrochromic materials for smart windows. Though electrochromism has long been studied; and is now somewhat mature, this group also conducts exploratory work on the formation and oxidation processes of nanoparticles, the photocatalytic action of TiO<sub>2</sub>, and photonic bandgap properties of Si-SiO<sub>2</sub> multi-layers (C. G. Ribbing), providing very good/excellent contributions to these exploratory research fields.

As for ZnO, TEM studies by Eva Olsson (Microscopy and Microanalysis, CTH) have disclosed details of the boundary structure in ZnO varistors, a classical device, whereas the potential of Mn-doped ZnO for spintronics is explored at Linköping University and at KTH (Applied Materials Physics, Börje Johansson). Quite recently, the reproducible formation of ZnO pn junctions and the successful emission of blue light have been reported by a Japanese group (M. Kawasaki). Related work on ZnO nanowires and nanorods has recently been performed by Magnus Willander at Physical Electronics and Photonics, CTH. In this case, the accumulation of insights via careful and continuous investigation is highly desirable.

Finally, a few additional comments are made on two important trends. Firstly, progress in the theoretical understanding of defect states and impurity states in chalcogen-based compounds has disclosed their potential. Theoretical work on vacancies in CuInGaSe solar cell structures by Börje Johansson's group (KTH) is one such example. Secondly, the ongoing progress in oxide semiconductor research is likely to expand this field in such a way that the area is eventually connected seamlessly with those of oxide dielectrics and superconductors, as suggested by the work of Per Delsing (Quantum Device Physics, CTH), Lars Hultman (Thin Film Physics, LiU), Alexander Grishin (Condensed Matter Physics, KTH), and others.

### *Quantum wells, layered Nanostructures and Surfaces*

Surfaces and interfaces of semiconductors exhibit various properties not seen in bulk systems. Spectroscopic studies on semiconductor surfaces and interfaces have been actively pursued by quite a few groups in Sweden. For example, Hans Siegbahn and Håkan Rensmo (Electron Spectroscopy and Molecular Surface Physics, UU) clarified the unique behaviour of photocatalytic TiO<sub>2</sub> and dye-sensitised ZnO-based solar cells, and Ulf Karlsson (Materials and Semiconductor Physics, KTH) disclosed new aspects of charge accumulation on InAs surfaces. Moreover, reaction processes on the surfaces of Si, Ge, InAs, and GaN have been investigated by Mats Göthelid, whereas Si layers buried in GaAs have been studied by Per-Olof Nilsson and co-workers (CTH). Since most of this work is already covered in the Surface Physics section, only the research activities on semiconductor layered nanostructures, bound by interfaces or surfaces, are briefly described here, although related accounts are separately given in the Nanoscience section.

As stated earlier, ("Quantum wells, ...") electrons and holes confined in quantum wells (QW's), ultra-thin FET channels, and other layered nanostructures play extremely important roles both in semiconductor physics and electronics. Moreover, these systems are also patterned to form quantum dots and wires.

To prepare these 2D systems, epitaxial growth methods, such as MOCVD, MBE, and chemical beam epitaxy (CBE), are used extensively. In major Swedish universities, intense activity has been directed to these core epitaxial techniques, putting them in a leading position in the field. In Sweden, these techniques have been amply exploited, of course, to grow GaAs/AlGaAs and other standard 2D systems, commonly used for physics research and device studies; they have also been modified and expanded to grow various exploratory quantum wells (QW's) and layered structures. Pioneering work on the epitaxial growth of various nitrides by Bo Monemar's group (Materials Science, LiU), and leading work on the growth

of SiC and SiGe in Linköping and KTH, are some examples. Moreover, some of these epitaxial methods have been ingeniously expanded by Lars Samuelson (Solid State Physics, LU) and others to form a variety of unique self-organised quantum dot and wire structures.

Although the physics of 2D electrons and excitons confined in GaAs/AlGaAs QW's, superlattices, and selectively doped heterojunctions, have been extensively studied for more than 30 years, there are still quite a few unsettled fundamental physics problems, especially when they are placed in strong magnetic fields to produce one of the quantum Hall systems (QHS's). The work of Hans Hansson (Fields and Particles, SU) and his partners on the polarisations and textured edges in QHS's is one example of such activities. The interaction of a spin-polarised edge channel with nuclear spins of Ga and As atoms is currently another hot subject of the field, but is little studied in Sweden.

A large number of research projects are being conducted on transport and the optical properties of 2D electrons and excitons in GaN-based and SiGe-based QW's, as well as their device applications. Typical examples are the efforts produced by the groups of Bo Monemar (LiU), Nils Nordell (KTH), and Thorvald Andersson (CTH) to explore the use of GaN/AlGaIn heterostructures for high-speed transistors (HEMT's), LED's, and inter-subband transition (ISBT) photonic devices.

### ***Quantum Wires, Nanotubes, Organic Semiconductors, and Related Structures***

Currently, a number of research groups in Sweden investigate various aspects of quantum wires (QWR's) and semiconducting nanotubes (NT's), as mainly described in the "Nanoscience and Nanotechnology" section and partly in the "Condensed Matter Theory" section of this report. Transport properties of semiconducting polymers have some features common to those of QWR's and NT's, as mentioned in the "Soft Condensed Matter" section of this report. Hence, only brief accounts are here made of a few specific activities.

As earlier described, semiconductor quantum wires have been prepared in Sweden not only by the top-down approach based on electron beam lithography, but also by a variety of bottom-up methods. One of the most unique and successful methods employed at present is perhaps the CBE or MOCVD growth of 10 nm-scale InAs and other III-V nanowires in selected spots on a substrate, where gold nanoparticles have been placed beforehand. This approach was first reported by a Hitachi group around 1992, but its rich potential has been disclosed only recently by a series of outstanding results from Lars Samuelson's team (LU) and Charles Lieber's team at Harvard.

This approach is truly a technical breakthrough, as it allows one to reduce the wire diameter to 10 nm or less, and also to passivate the wire by coating its surface with other materials. Indeed, by making use of such an InAs quantum wire, a novel field effect transistor (FET) has been fabricated, in which the current is carried by quantised one-dimensional electrons. More importantly, this approach enables one to modulate both the material composition and the potential profile  $V(x)$  along the wire axis, and, thereby, allows quantum control of 1D electrons. Indeed, a pair of InP barriers has been successfully introduced, with a tiny quantum dot (QD) in between, to demonstrate resonant tunnelling transport. In addition, coupled QD molecules and other unique nanostructures have been formed; and their surprising properties demonstrated. To these QWR studies, high-resolution TEM investigations by Reine Wallenberg (Materials Chemistry, LU) have made significant contributions. This method of nanofabrication will surely create a huge impact, as it allows one to form a variety of novel nanostructures, including those quite suitable for single photon emitter, qubits, and quantum gates, as will be mentioned in subsection "Quantum dots ...".

Depositing materials selectively in the bottom region of a sharp groove structure can form III-V QWR's of another kind. In collaboration with EPFL researchers, H. Weman (Materials Science, LiU) has made notable contributions to upgrade the performance of such QWR lasers and to demonstrate the feasibility of QWR optical modulators, based on the confined Stark effect of 1D excitons.

Quantum point contact (QPC) devices are normally prepared by e-beam lithographic patterning of a high-mobility 2D electron gas system in an n-AlGaAs/GaAs heterojunction. The QPC is, in a sense, the shortest limit of a quantum wire, although care is needed to pay attention to its unique situation. It has been reported that the first step of quantised conductance, associated with the ballistic transport of 1D electrons in the ground subband, is often accompanied by an anomalous structure, called "0.7-conductance anomaly". The possible origin of this anomaly has been discussed by Irina Yakimenko and Karl-Fredrik Berggren (Theory and Modelling, LiU), who tentatively ascribe it to a kind of spin-polarisation effect.

Certainly, more theoretical work is needed to clarify the roles of various interactions of "quasi" 1D electrons both in long and short QWR structures. In fact, very good/excellent theoretical work has been conducted by Stellan Östlund and Henrik Johannesson (Solid State Theory, CTH) on the Tomonaga Luttinger liquid aspects of QWR's, which will hopefully be followed by some experimental work.

Various Si quantum wire structures have been produced and their reliable FET actions demonstrated by quite a few groups, including that of Shi-Li

Zhang (Materials and Semiconductor Physics, KTH). They are mostly made by performing electron beam patterning and subsequent etching and oxidation processes on Si MOS FET's on SOI substrates. Note that these methods are quite close to the standard fabrication process of advanced MOS LSIs. Since ultra-small QWR MOS FET's are one of the attractive structures for future LSIs, and also one of the clean model 1D electron systems, they should be thoroughly studied.

Carbon nanotubes (CNT's) can be metallic and semiconducting, depending on their chiralities. Growth mechanisms of CNT's, particularly those at selective spots on Si substrates, have been studied by Eleanor Campbell's group (Atomic Physics, CTH/GU) in a very interesting collaboration with the TEM group of Eva Olsson (Microscopy and Microanalysis, CTH/GU); they have also been successful in promoting exploratory research for their applications, including as a field emission source of electrons, novel nanorelay devices, FET's and other devices. Bertil Sundqvist's group (Experimental Physics, UmU) has conducted a series of excellent experiments on  $C_{60}$  and CNT's, and discovered quite unique (magnetic) properties of  $C_{60}$  molecules formed by the cross-linking of  $C_{60}$  under very high pressures. This group explores new properties of CNT "peapod" structures, which contain a number of fullerenes inside. Anna Delin (Applied Materials Physics, KTH) has used CNT's as a cage to house a string of ferromagnetic nanowires. This approach is somewhat similar to the work of Osamu Terasaki (Inorganic Chemistry, KTH), who utilises nanoporous zeolites to form a variety of nanostructures.

Organic semiconductors, both polymer and oligomer molecules, have been intensively studied in recent years because of their importance in physics and device applications, as stated in the Soft Condensed Matter section of this report. In the Center of Organic Electronics (LiU), W. R. Salaneck has performed photoelectron spectroscopy and has obtained important insights into the energy line-up of relevant HOMO/LUMO levels at organic heterojunctions and electrodes, which strongly affect the performance of polymer light emitting diodes (LED's). Olle Inganäs (Biomolecular and Organic Electronics, LiU) has worked on several key unresolved issues, as future prospects of organic solar cells and lasers depend on them. Thorvald Andersson (Microwave Electronics, CTH) has started research on oligomer-based organic LED's by using his expertise in molecular beam (vacuum) deposition technique. In contrast, transport properties of organic semiconductors have attracted strong attention for their FET applications, as well as for their basic academic interest. For example, high-mobility carrier transport phenomena in novel PPV- $C_{60}$  composite systems, and the possibility of resonant tunnelling via DNA molecules, have been theoretically studied by Sven Stafström (Theory and Modelling, LiU). Carrier transport through a single organic

molecule is another hot subject; Göran Wending (Applied Quantum Physics, CTH) has theoretically shown that such a single molecule transport is critically influenced by the contact resistance, as it depends on the precise geometry of a molecule – electrode contact. Indeed, the importance of contacts is now very well noted in recent experimental studies.

### *Quantum Dots and Semiconducting Nanoparticles*

At present, a good number of researchers in Sweden work on various aspects of quantum dots (semiconducting nanoparticles), as mainly described in the “Nanoscience and Nanotechnology” section and partly in the “Condensed Matter Theory” section of this report. Hence, only a few specific projects are briefly mentioned here. A brief account is also given of a class of organic semiconductors made up of oligomers, as carriers (mainly holes) are pretty much confined in each organic oligomer molecule; and intermolecular transport is somewhat similar to inter-dot transport. For the other class of organic semiconductors consisting of polymers, intra-molecular quasi-1D transport process play a critical role, as described in the “Soft Condensed Matter” section of this report.

As stated before, quantum dots can be formed in a number of ways; in particular, electron beam lithography and the Stranski-Krastanov growth of self-assembled dots have often been used. Swedish researchers have not only exploited these methods extensively, but have successfully developed a couple of unique methods and disclosed their potential. For example, Lars Samuelson’s team (Solid State Physics, LU) has ingeniously refined the selective growth process of semiconductors on particular spots, which are covered by Au nanoparticles beforehand; they have demonstrated that this approach enables one to form both uniform nanowires and compositionally modulated wire-like structures, in which quantum dots and barriers can be arbitrarily embedded. The same approach has recently been used by Magnus Willander (Physical Electronics and Photonics, CTH) to make ZnO nanorods. Some years earlier, Samuelson’s group also developed a vapour phase method to form aerosol (nano) particles of semiconductors. Nanoparticles thus formed are placed on a substrate and manipulated by an STM/AFM tip to sit between a pair of electrodes in order to form a novel single-electron transistor. Mamoun Muhammed’s group (Materials Chemistry, KTH) has extended the controllability of the solution chemistry approach and successfully formed ZnO and other nanoparticles for a variety of applications.

The discrete states of a quantum dot with many confined electrons can get quite complicated, especially when exchange and correlation energies play important and sophisticated roles in the presence of magnetic fields. S.M. Reimann (Mathematical Physics, LU) has made an excellent analysis of

such systems theoretically and clarified features of the shell structure; she has also examined and disclosed novel magnetism in a QD lattice system.

Concerning the electron transport through a single or multiple QD's, Karl-Fredrik Berggren and his co-workers (Theory and Modelling, LiU) have conducted theoretical work on chaotic trajectories of electrons in an open quantum dot (billiard), while the Solid State Physics group (LU) disclosed both experimentally and theoretically unique features of quantum ratchet mechanisms that can be realised in an array of asymmetric open QD's. Moreover, by introducing a pair of tunnel barriers into a quantum wire structure and by forming a quantum dot or a rod-like island structure in between, Lars Samuelson's group has succeeded in making a novel high-performance single-electron transistor (SET) and a novel double barrier resonant tunnelling transistor. Note that the constricted Si MOS FET, having a quantum point contact (QPC) geometry, is found to exhibit excellent SET characteristics even at room temperatures, indicating the unexpected formation of a double barrier structure with a tiny QD in between.

Some pioneering work has been performed by a couple of Swedish research groups on the photonic properties of quantum dots; for example, Lars Samuelson's group (LU) has conducted single dot spectroscopy of an InAs QD and clarified the role of neutral and charged excitons as well as bi-excitons, which are formed under high-excitation conditions. Similarly, Per Olof Holtz (Materials Science, LiU) and his collaborators have performed excellent single dot spectroscopy on InAs QD's by using dual laser excitations, and clarified the roles of many body effects of excitons and carriers. He studied with Göran Hansson (Surface and Semiconductor Physics, LiU) and Wei Xin Ni (Materials Science, LiU) the optical transition processes in Ge QD's, where electrons and holes can be placed both in spatially direct and indirect geometries. Kung-An Chao (Solid State Theory, LU) has conducted a theoretical analysis of polaron effects in QD's, which are found to play important roles in the relaxation process of carriers in QD's, as well as interpreting the inter-subband spectroscopy of InAs QD systems.

The impact of quantum dots is not restricted to electronics and photonics alone, but is also expected to extend to the biomedical and ecology areas, as illustrated, for example, by the use of  $\text{TiO}_2$  nanoparticles, as photocatalysts. One should also note that various organic oligomers,  $\text{C}_{60}$  molecules, and peapod structure in CNT's studied by Bertil Sundqvist (Experimental Physics, UmU), are also quite important.

### ***Device Studies and Related Techno-Scientific Research***

Research activities on semiconductor devices cover a wide spectrum of subjects, ranging from those directly related to well-developed Si LSIs, all

the way to highly exploratory efforts on quantum computation. Since most of these activities have already been described in earlier subsections, we here briefly state representative activities, and also provide some detailed comments on the activities of a couple of specific groups.

As stated in subsection “Si, SiGe, SiC, C, and Related Materials”, the science and technology of Si-based LSIs are approaching a stage of maturity, or the region of a “red brick wall”, where further advances are likely to be mainly made by the clever use of nanostructures and/or new materials other than Si and SiO<sub>2</sub>. The use of high k dielectrics and ferroelectrics in place of SiO<sub>2</sub> is one example, as attempted by Alexander Grishin (Condensed Matter Physics, KTH). KTH and LiU have conducted quite active research and made interesting contributions to

SiGe-based hetero nanostructures, while their work on Si-based nanostructures has remained comparatively less. Another area of importance for silicon is the field of power devices, such as IGBT’s and thyristors, which will play indispensable roles in future energy systems. Pioneering work on SiC materials and devices done by Swedish researchers (described in subsection “Si, SiGe, SiC, C, and Related Materials”) will play an increasingly important role.

Currently, III-V compounds are used widely in high-speed transistors and photonic devices. In any wireless and fibre communication systems, high-speed transistors (HEMT’s and HBT’s), made of GaAs/AlGaAs and InGaAs/InP heterostructures, are routinely used. Specialists expect that GaN/AlGaN HEMT’s, when appropriately developed, may well replace some of these devices, and will be used as high-speed high-power transistors operating in base stations of future wireless systems. As Swedish research groups at LiU, KTH, and CTH conduct extensive studies on nitrides, and some of them, especially Monemar’s group (LiU), have played leading roles in this field, (as noted in subsection “The III-V compounds ...”, and below), their future contribution to this subject could be quite significant. Another and more important application area of nitrides is blue and UV LED’s and lasers, which are used for full-colour displays, lighting, high-density optical discs, sterilisation, etc. Moreover, as stated in the section “The III-V compounds...”, novel nitrides, such as GaInNAs (with very low N content) and InGaN (with very high In content), can potentially be used as small bandgap materials, suitable for fibre communication devices. Because of the leading role that some Swedish research groups have played up to now, their substantial contribution to this important field is to be expected. In order to supplement our rather general statements on nitride device research, some specific comments will be provided in the following paragraphs on activities of two device research groups, led by Magnus Willander (Physical Electronics

and Photonics, CTH) and Thorvald Andersson (Microwave Electronics, CTH), since their activities on nitrides are only briefly stated in subsection "The III-V compounds...".

The physical electronics and photonics group of Magnus Willander conducts research on an exceptionally large number of subjects, covering, for example, growth and optical investigations of arsenides (InAs quantum dots and GaAs/AlGaAs quantum wells), nitrides (GaN, AlGaN, and GaInNAs), and novel ZnO nanorods, as well as exploratory works on the control of molecules and ions in water-based systems. The group, despite its limited manpower, has promoted numerous projects in parallel; and continued to provide a variety of rather interesting findings, such as the selective growth of high-quality ZnO nanorods using Au nanoparticles. Although the group is quite productive as it is, the concentration of research efforts on a smaller number of selected subjects is likely to raise the overall quality of its research activities and enhance its contribution to the scientific community.

The Microwave Electronics group of Thorvald Andersson (CTH) is one of the first in Sweden to initiate molecular beam epitaxy (MBE) studies to grow III-V semiconductors for transistors and photonic devices. At a very early stage, they studied the growth of lattice mismatched InGaAs/GaAs systems and clarified morphological changes of the InGaAs layer into quantum dots and/or a dislocated layer. Recently, they focused on the MBE growth of GaN and related nitrides, important for both blue light emitters and high-power microwave transistors. Although nitride devices are now produced mostly by MO CVD, MBE studies done in CTH and elsewhere have provided complementary insights into growth mechanisms, such as In segregation in InGaN films, the impurity incorporation and interface roughness in GaN/AlGaN systems, and the growth of GaN/AlN on silicon. These MBE activities on nitrides are good and effective in providing understanding of sophisticated growth mechanisms of nitrides that are complementary to those obtained by very active MOCVD studies conducted in Linköping and elsewhere. This group has begun MBE studies of organic semiconductors for LED applications, as briefly stated in the section "Quantum wires ...".

Apparently, the field of semiconductor device research is quite diverse and extends far beyond those subregions represented by Si-based LSIs and power devices, and III-V based lasers and IT devices. In this paragraph and the next, some Swedish research activities on more exploratory devices will be described. For example, various emitters and detectors for the spectral region of the mid-infrared (MIR) and THz have been studied. Quantum well infrared photodetectors (QWIP's), which make use of the photoconductivity induced by the inter-subband transition (ISBT) of electrons in quantum wells, were

ingeniously refined by KTH scientists to reach the level of a commercial product. Recently, the extended use of ISBT processes in GaN QW's is being explored by Nordell's group (Materials and Semiconductor Physics, KTH), whereas the ISBT process in SiGe QW's is studied by Roger Uhrberg, Göran Hansson, and Wei-Xin Ni (Surface and Semiconductor Physics, LiU) to make a novel MIR emitter (quantum cascade laser). Koung-An Chao (Solid State Theory, LU) has examined theoretically THz-gain mechanisms for the Bloch oscillation in superlattices. These devices may well play an important role in high-resolution gas sensing and MIR/THz imaging, key technology in ecological and medical diagnosis.

Novel devices based on unique interactions of semiconductors with blackbody (thermal) radiation have also been investigated. For example, a new IR bolometer that makes use of the ultra-high temperature sensitivity of Mn oxides is demonstrated by Alexander Grishin (Condensed Matter Physics, KTH). A new scheme for opto-thermionic refrigeration is proposed and theoretically analysed by Koung-An Chao (LU), whereas the UV absorber characteristics of ZnO nanoparticles have been successfully controlled by Mamoun Muhammed (Materials Chemistry, KTH) for thermoelectric applications.

Chemical interactions of semiconductors have also been explored in relation to device research. For example, the catalytic action of metal oxide nanoparticles, such as TiO<sub>2</sub>, has been studied both by M. Muhammed's group (KTH) and by Granqvist's group (Solid State Physics, UU). The influence of hydrogen in various MIS systems, such as Pt or Pd electrodes on SiO<sub>2</sub>-clad SiC, has been studied by I. Lundström/M. Eriksson (LiU) for gas sensor applications.

In recent years, exploratory research has been intensively promoted on various devices useful for quantum computing systems and/or for quantum cryptographic systems. Indeed, a variety of approaches to build qubits has been proposed; for example, both charge qubits and flux qubits based on Josephson junction SET/SFQ circuits have been proposed and demonstrated; Per Delsing's group (Quantum Device Physics, CTH) has made noteworthy contributions to this field. Similarly, both charge qubits and electron spin qubits based on coupled semiconductor quantum dots (QD's) have been proposed and demonstrated, in which the decoherence time of such qubits has been clarified. Others have proposed to build qubits by using nuclear spins of impurity atoms in Si and also of Ga and As atoms in GaAs.

Stefan Kröll's group (Atomic Physics, LU) has made an attractive proposal to form qubits by using the nuclear spins in (interacting) RE ions embedded in inorganic materials. Although this proposal is conceptually sound, the prospects for this approach appear to depend on whether or not these rare

earth ions can be introduced as intended. Hence, the real potential of this proposal will only become clear when one elucidates the ability to control the exact positions of RE ions and their spacing. In fact, it is often said that quantum information technology must be developed in order to transfer the quantum state of light into that of electrons, and the quantum state of such electrons should be transferred to that of nuclear spins. Hence, it is perhaps quite meaningful to continue parallel research efforts on various qubits. S. Kröll's group has carried out excellent work on quantum manipulation of photons; the work includes the reconstruction of quantum state of a single-photon wave packet in a Doppler-broadened transition, as well as delayed self-interference of single photons.

Apart from quantum computation, numerous attempts have been made to control spins; for example, spin injection in (CdZnMn)Se has been studied by Irina Buyanova and Weimin Chen (Materials Science, LiU). The spin-LED action of GaMnN/GaInN systems has been demonstrated at room temperature. The possible control of the spin current in an AB loop, and also optoelectronic spin injection, has been clarified.

### *Theoretical Activities and Topics*

Undoubtedly, research activities in Sweden at the forefront of semiconductor physics have mostly been promoted by collaborative efforts of both experimentalists and theorists. It is especially true in those areas in which many-body interactions, quantum confinement, and localisation of electrons play important roles. Since most of the theoretical work is described systematically in another section of this report, only a few representative topics relevant to semiconductor research are briefly mentioned here.

Quite interesting aspects of electronic states in various quantum dot (QD) systems, including QD lattices, quantum billiards, and rings, have been disclosed by theoretical groups such as those of S. Reimann (LU), Igor Zozoulenko/Karl-Fredrik Berggren (LiU), and Leonid Gorelik (CTH). Unique features of the Luttinger-Tomonaga (LT) liquid behaviour of interacting one-dimensional electrons in quantum wires (QWR's) have been disclosed by several groups, including those of Igor Abrikosov and Irina Yakimenko (LiU), and of Stellan Östlund and Henrik Johannesson (CTH/GU). Exchange interactions in ballistic QWR's have been discussed in connections with the 0.7 conductance anomaly (Yakimenko/Berggren).

Another interesting piece of work is being conducted by Hans Hansson's group (KTH) on the composite Fermion theory of half-filled Landau level in quantum Hall systems (QHS). In view of the continuing high level of experimental activities going on globally, a somewhat higher level of theoretical work on QHS is to be desired.

As for semiconductor-based spintronics, various noteworthy theoretical programmes are underway; they include the study of GaMnAs by Olle Eriksson (UU), the analysis and control of the Rashba effect (Ulf Ekenberg, KTH), and spin-polarised electron injection in II-VI heterostructures by Koung-An Chao (LU). In view of the interdisciplinary nature of this field, cross-border interactions of researchers with those of neighbouring fields, such as Anders Rosengren (KTH), and many others working on strongly correlated systems, would be meaningful.

## Future Perspectives

It is almost an impossible task to predict future developments of academic research in any field of science. This is mainly because the advent of an unexpected discovery, a technological breakthrough, and/or a ground-breaking concept can significantly change the landscape of a specific field and affect the course of progress thereafter. Nonetheless, it is still of some use to examine the past trends of semiconductor research and discuss a couple of promising directions through which new and key developments are likely to emerge. Generally, it can be safely said that new findings are likely to be gained when explorations are made on new semiconductor structures, new semiconductor materials, as well as new phenomena and new functions of Semiconductors, as will be examined below.

As already discussed in the subsections “Nanostructured Semiconductors and Surfaces” and “Quantum wells..., Quantum wires..., and Quantum dots...”, one important frontier of semiconductor studies is the field of man-made nanostructures, in which low-dimensional electrons and excitons exhibit a variety of new and remarkable properties and functions. As stated in the previous section, most of the Swedish universities are actively engaged in this field. Indeed, a good number of Swedish research groups have conducted very high-quality research, and some of them have made outstanding contributions to this field. It is now widely recognised that this field is important not only for pure and applied physics, but also for other branches of science and engineering. Hence, it is highly desirable to maintain active research activities in this trans-disciplinary field, particularly by enhancing the interaction of physicists with chemists, materials scientists, biologists, physicians, electronic engineers, and other scientists in related fields.

Another challenging subject in semiconductor studies is the exploration of new physical phenomena and device functions that are relevant to quantum information processing. As earlier stated, various attempts have been made to form qubits by making use of electronic charges or spins in coupled quantum dot systems. A couple of methods to control nuclear spins in semiconductors

for the possible realisation of qubits have also been investigated, both in doped silicon and in GaAs-based quantum Hall systems. In addition, various new photonic devices, including single-photon emitters and detectors, have been developed to enable secure quantum key distribution in quantum cryptographic systems. Although no one can tell when, and how, a useful quantum computer can be realised, and what sort of impact this will have, it is still quite valuable to promote long-term research activities in these areas to clarify, for example, how the coherence of a particular quantum state is lost and how the entangled states can be generated – as they are important and represent fundamental issues in basic condensed matter physics.

As discussed in the previous two sections, new semiconductor materials, such as GaMnAs and other emerging systems, have exhibited a variety of novel physical properties, which mainly result from many-body effects in semiconductors. Note also that SiC, ZnO, InAlN, TiO<sub>2</sub>, Alq<sub>3</sub>, and some other systems, although being long known by name, have just started to disclose most of their inherent properties, since methods to control the quality of these materials have become available only quite recently. As the majority of this work is still at an exploratory stage, one should keep exploring these research fields until their physics and device potential are fully disclosed.

By contrast, Si, Ge, GaAs, and other materials widely used in semiconductor devices have been well studied. These systems will still play a significant role in future CMP research, as they can be prepared with extremely high purity and also can be processed into a variety of nanostructures, heterostructures, and device structures, including nano-electro-mechanical systems (NEMs) and micro-fluidic systems, which may open up new fields of research. Moreover, the interaction of exploratory condensed matter physicists with device specialists at the technological cutting edge has been, and will be, quite fruitful for both sides.

Technological and scientific methods for micro- and nanostructure fabrication, such as epitaxial growth techniques and nanolithography developed originally for semiconductor devices, have opened important passages not only to advanced electronics, but also to the entire field of nanoscience and technology. Hence, efforts at major Swedish universities to keep and make the best use of micro- and nanoprocessing capabilities for basic research should be viewed positively. Of course, the cost effectiveness of these facilities should be monitored to establish sustainable systems, as the cost and the manpower for running such facilities can be rather high. It may be worthwhile investigating how other countries deal with this universal problem, including the recent effort of the NSF in the USA, which has organised a national consortium of more than ten universities for the promotion of nanotechnology research.

Finally, some comments will here be made on the a delicate issue of how to achieve a good balance between the freedom and independence of individual researchers and the co-ordinated group efforts often needed to perform top quality experimental studies of semiconductors. One recipe, often used in the past in continental European countries, is to appoint, with care, an outstanding full professor with excellent vision and leadership, and to provide him/her with enough posts and power to form, and run, a research group that is large and stable enough to allow the accumulation and concerted utilisation of the technical skills needed in experimental studies. Another recipe, often used in some US universities, is to form a number of relatively small research groups with ample freedom and independence, and then promote various inter/intra university collaborations based either on the researchers' own initiatives or under the leadership of department heads, deans, and funding officers. Some of Swedish universities appear to be halfway between the two, as they intend to make transitions from the former style to the latter. In-depth examination and discussions are needed to find the optimum systems for Swedish universities.

## Superconductivity

### International Perspective

Since the “Annus Mirabilis” of 1986, superconductivity is, independent of any current or future applications, still a very important area of basic research with many unanswered questions, and with a future potential for discoveries and progress in various directions. Fundamental research in high- $T_c$  superconductors (HTSC), because of the complexity of the materials, brings together theoretical and experimental expertise from physicists, chemists, materials scientists, electronic engineers, etc. Microstructure, crystallinity, non-equilibrium phases, and overall dimensional and structural issues play a crucial role and can strongly affect the physical properties of the materials.

Before evaluating the superconducting activities in the Condensed Matter Physics Community of Sweden, we first give a brief overview of the current activities and possibilities in the fields of theory, experiment, and techniques.

### Theory

Since the discovery of high- $T_c$  superconducting materials, many ideas have been put forward to explain their unusual physical properties. Rather than attempting to survey the field, we will briefly discuss three perspectives: the

phenomenological approach; numerical studies of Hubbard and t-J models; and electronic structure.

The cuprates are highly correlated systems close to the Hubbard-Mott antiferromagnetic insulating state. In the optimally doped case, generalisations of techniques developed for ordinary superconductors may be applicable with appropriate modifications. An important issue for the future is to extend the calculations to the underdoped regime, where pseudogap signatures go well beyond the classical metallic behaviour. There is however, as yet, no systematic quantification of pseudogap effects, and contrary views exist as to their origin. In the preformed pair model the pseudo- and superconducting gap have a common origin with the superconducting transition being related to the onset of phase coherence. In this framework, an important aim for the future should be to achieve a common understanding of ARPES, optical and tunnelling data simultaneously.

Numerical studies of the high- $T_c$  cuprates have been used to determine what types of correlations are significant in specific models. They have shown that the 2D Hubbard and t-J models exhibit antiferromagnetism, striped domain wall and d-pairing correlations. The similarity of this behaviour to the phenomena observed in the cuprates supports the notion that the Hubbard and t-J models contain essential physics of the HTSC problem. A key issue is to determine whether the underlying physics is to be understood in terms of spin-charge separation, stripes, spin-fluctuation exchange, or whether additional phonon-mediated interactions may play a supporting role.

The discovery of superconductivity in  $MgB_2$ , and the response by the computational community, has demonstrated the remarkable progress that has been achieved in first-principle calculations of the electronic properties of conventional (phonon mediated) superconductors. Indeed, the electron-phonon spectral density,  $\alpha^2F(\omega)$ , can be calculated accurately for fairly complex materials using density functional methods. Not only can the electron-phonon coupling be obtained, but also complete phonon dispersion curves for the whole Brillouin zone are being calculated using perturbation theory. There are many questions, which are now approached with model Hamiltonians. There is, however, a strong desire to develop the apparatus required for a real first principles treatment of the HTSC phenomena.

## Experiments

New systems can be found by either bulk or thin film methods, each of which has its advantages, disadvantages, challenges, and opportunities. The search for new materials has always been, and remains, an important area of research in the field of superconductivity. Also important for the develop-

ment of potentially practical materials and the understanding of the complex physical phenomena, which occur in superconducting materials, has been the use of chemical doping or manipulation in order to influence the electronic and magnetic properties of the superconducting systems. Undirected combinatorial chemistry will never get through the entire possible range of element / treatment combinations in a search for superconducting materials; some materials physicists have used the “phase spread method” with success.

Because of the large coupling between charge, spin, and lattice in the HTSC and other transition metal oxides, doping of these materials with charge carriers can also be accompanied by the formation of static and dynamic spin and/or charge ordered phases on a microscopic scale. These “stripe phases,” have recently been observed in many perovskite-based transition metal oxides, including several cuprates, and may be a general feature of those systems. Achieving a comprehensive understanding of spin/charge self-organisation in oxides is a challenging task. The details of the effects of atomic substitution or doping are not yet fully understood in the HTSC, and this represents an active area of current research.

There seems to be much work needed to understand in detail the connections, control, and effect of defects on HTSC. This is important for applications, particularly those that require high critical currents such as power applications. We are still far from understanding, or being able to optimise, HTSC material properties in the way that we have learned to do for the workhorse conductors NbTi and Nb<sub>3</sub>Sn of low-T<sub>c</sub> superconductors (LTSC). Some of the remaining key issues derive from the anisotropic nature of the cuprates and their low carrier density. These characteristics result in inadequate magnetic flux pinning, percolated current flow past many interfacial barriers, inability to control the phase state, and a general lack of materials control.

Most of the electromagnetic properties of Type II superconductors are determined by vortices in static and dynamic configurations. Rapid progress in manipulating and measuring vortices in recent years has greatly expanded the limits of known and imaginable vortex phenomena. Individual vortices in an array can be manipulated by imposing an artificial mesoscopic template. There are fascinating possibilities in hybrids composed of magnetic dots deposited on a superconducting layer. Here the magnetic dot is a magnetic flux pin site that is isolated from the superconductor. Unlike LTSC's, the cuprates have clearly defined lattice, liquid, and glassy phases that will react quite differently to the imposed order of the template. The liquid and glassy states of multi-vortex matter offer major challenges for understanding the magnetic properties of superconductors. The vortex liquid shows equally

fascinating behaviour arising from thermal disorder rather than quenched disorder.

Many fundamental studies and a large number of applications require the HTSC materials to be in proximity with other materials. Thus, issues of proximity effects, spatial variations close to an interface or surface, and structural and materials variations are particularly important in thin film and/or nanoscopic structures. The very short coherence lengths characteristic of high- $T_c$  materials make them much more susceptible than LTSC to the influence of neighbouring materials and internal defects, virtually at the atomic level. Understanding the proximity effect is a critical element in the study of the high-temperature superconductors.

Research in the electronic properties of HTSC has proved to be particularly interesting and fruitful. The improvement in real and reciprocal space resolution has uncovered many interesting properties. However, it is not clear whether these properties are essential in superconductivity. It also seems that competing phenomena are present in most HTSCs. It is therefore interesting to investigate systems that form instabilities, such as the metal-insulator transition, magnetic phases, electronic instabilities such as stripe phases, etc. Comparison of classical infrared spectroscopy, and photo-emission measurements, may prove to be very fruitful. Issues such as surface contamination, surface segregation, and the general heterogeneity of the materials close to surfaces and interfaces must be addressed.

Advanced demonstrations of fundamental properties of engineered quantum systems consisting of LTSC superconducting Josephson junctions (JJ) circuits, representing qubits, have been made. The most promising solid-state qubits are based on JJ's; they take advantage of the intrinsic coherence of the superconducting condensate. The distant goal of quantum computers has focused a lot of attention on quantum state engineering and quantum measurement, areas in which substantial progress has been made.

### Techniques

New lithographic and preparation techniques allow modifications and confinement of superconducting materials on lengths scales approaching the superconducting penetration depth, and in some cases the coherence length. Moreover, novel imaging techniques have been developed, and these can give detailed microscopic images of the vortex system.

Electron tunnelling (both quasiparticle and Josephson tunnelling) has been a powerful technique to probe the excitation spectrum, the superfluid density, and the pair wave function phase of conventional superconductors. SPM studies offer an important additional feature that has already yielded some surprises. STM quasiparticle tunnelling has allowed both microscopy

and spectroscopy to be performed with good energy resolution and with the spatial resolution to study the gap parameter on a length scale smaller than the superconducting coherence length.

Angle-Resolved Photoemission Spectroscopy (ARPES) experiments have contributed to our understanding of the electronic structure and superconducting properties by revealing information on the Fermi surface, and a large superconducting gap anisotropy that is consistent with a d-wave pairing state. It should be remembered that both ARPES and tunnelling are surface probes. Inelastic X-ray Scattering (IXS), which is not sensitive to surfaces or defects, is a valuable probe of bulk states. Infrared and optical spectroscopy is ideally suited for studies of superconductivity because of the ability of these techniques to probe such fundamental parameters as the energy gap and the superfluid density.

Considerable knowledge of antiferromagnetic and spin fluctuations in the cuprates has been obtained experimentally using neutron scattering, nuclear magnetic resonance (NMR), and muon spin rotation ( $\mu$ SR) spectroscopy. The phenomenon known as “stripe” order has been observed by neutron and X-ray diffraction in several variants of the HTSC family. There are many unresolved issues associated with the problem of competing orders in stripes. Studies with a wide range of techniques will be needed to answer these questions.

### Conclusion

There is still much work needed to understand in detail the control and effect of defects, interfaces, nanostructures, etc. on high- $T_c$  as well as low- $T_c$  superconductors. This, of course, is very important for applications, particularly those that require thin film and tunnel junction preparation for electronic systems, or high critical currents for power applications.

Much of the research in high- $T_c$  superconductivity has spilled over to other areas of research where complex materials play an important role, such as magnetism in the manganites, complex oxides, two and three-dimensional magnetic devices, etc. Applications could greatly benefit from the discovery of new superconductors, which are more robust and which can be more easily manufactured.

## Superconductivity in Sweden

### Theoretical Activities

At CTH, the Applied Quantum Physics group consists of Vitaly Shumeiko and Göran Wendin, who work closely together, and Mikael Fogelström

(Ph.D. in 1995), who joined the group quite recently and so far appears to be working independently, although on related topics. The strength of this group is in superconductivity, Josephson junctions, and related physics. They do primarily analytic theoretical work based on techniques, such as perturbation theory, as well as proposing new devices. Shumeiko and Wendin have focused on the theory of candidate solid-state qubits. They have suggested a new type of superconducting qubit based on an Andreev bound-state localised near a quantum point contact. They have also studied a mechanism for read-out from a standard superconducting quantum dot, the “Cooper-pair box”, in which two states of qubit differ by the addition of one Cooper pair to a superconducting grain. Their proposed read-out mechanism involves a single-electron transistor (SET) capacitively coupled to the Cooper-pair box. In collaboration with the experimental group of Per Delsing (Quantum Device Physics, CTH), they concluded that the SET could be used to read out the Cooper-pair box in a single shot. Another part of their activity concerns artificial grain boundary junctions of HTSC, motivated by the experimental evidence of d-wave symmetry of the order parameters. The present interests of the group, in some timely topics, are also offshoots of their expertise. Superconducting qubits are promising as well as risky areas with many interesting possibilities. This group is doing very good work on issues, which are both fundamental science, and of possible future technological importance.

Several senior members of the Condensed Matter Theory group at CTH work closely together – Mats Jonson, Robert Shekhter, and Leonid Gorelik – largely on projects in the nanoelectronics field. In particular, they proposed in 1998 an interesting shuttle mechanism for charge transfers in Coulomb blockaded nanostructures. They showed that transportation of Cooper pairs by a movable single Cooper-pair box placed between two remote superconductors can establish a coherent coupling between them. This work, which was led by Gorelik, is relevant to transport in nano-electromechanical (NEMS) single-electron transistors. Jari Kinaret (Ph.D. in 1992) works largely independently on somewhat similar problems, using more technical methods, such as the “Luttinger liquid” theory. His project focuses on the role of Coulomb interactions on the transport between two superconductors coupled through a quantum dot. Future activities of the group in superconductivity are centred on the possibility to set up a spin-controlled supercurrent. To this end, they will consider both Josephson currents through a normal 1D-channel and through a Cooper-pair box. This heterogeneous group of young and older researchers is carrying out some creative studies, which are timely and have both fundamental and applied aspects. This is an excellent group.

The Solid State Theory group at CTH/GU, headed by Stellan Östlund, consists of six senior researchers who, although they interact with each other, work in different subfields in condensed matter physics. One of them, Mats Granath (Ph.D. in 1999), is concentrating on the study of stripe formation in HTSC. Besides experimental evidence, there is also extensive numerical work on small Hubbard or t-J clusters, which indicate the presence of stripes. More recently, his analysis was extended to a broader range of charge ordered structures, including diagonal stripes, in-phase stripes, and bubble phases. Within his model, "staircase" stripes naturally reproduce the characteristics seen in ARPES. He is currently also pursuing ideas of the influence of electron – phonon interactions in the cuprates. One phonon in particular, an in-plane longitudinal optical Cu-O-Cu bond-stretching mode, has been found to couple strongly to the doped charge. His career is still at a relatively early stage, but it seems to be going in the right direction in view of the very good work performed up to now.

At the University of Skövde, Krister Karlsson (Ph.D. in 1992) studies the stripe phases in materials, such as hole-doped La and YBa compounds. The dynamical mean-field theory (DMFT) equations for the stripe phase obtained from the 2D Hubbard model are solved using an exact diagonalisation method. The aim of Karlsson's work is to study screening processes, as well as the formation and stability of different magnetic structures in the stripe phases of hole-doped cuprates. These studies will be pursued in collaboration with S. Biermann (Ecole Polytechnique, Paris) and F. Aryasetiawan (Tsukuba, Japan). Karlsson has a relatively short publication list, although it is difficult to use the same scale for rating individuals in smaller places, as for Olle Eriksson (UU), with whom he collaborates. The emphasis of his work seems, however, to be in magnetism, and it might be of interest to have more focus in future research activities. The Expert Panel encourages further support for individuals such as Karlsson, who continues to do very good research at a steady pace.

At Luleå University, Hans Weber studies superconducting vortex fluctuations in two and three dimensions. Both static and dynamic aspects have been covered, as well as the effect of disorder. He collaborates with a group at UmU (Petter Minnhagen and Beom Jun Kim) calculating critical exponents of the 3D Landau lattice model. In collaboration with S. Teitel (Rochester University, NY) and Mats Wallin (Condensed Matter Theory, KTH) he is involved in the study of columnar pins, made by shooting ions through a superconductor. Weber's research output appears to be less than average for Swedish condensed matter theorists. This may be explained by the lack of Ph.D. students and his currently high teaching load (75% funding). Nevertheless, this is a good activity in the field of superconductivity.

The Theoretical Physics group at Umeå University (UmU) consists of two subgroups whose activities are reported separately. The quantum theory group (Jörgen Rammer and Andrei Shelankov) has a broad range of research activities, such as the theory of superconductivity, the study of disordered systems, mesoscopic physics, etc. In the field of non-equilibrium superconductivity, thermo-electric effects have been studied. The theory of d-wave Josephson junctions was also considered in a series of papers. A unifying theme for large parts of their activities concerns quantum coherence in various contexts. Their future activities seem to be much less (or perhaps not at all) related to superconductivity. The recent very good work of the statistical group of Peter Olsson (Ph.D. in 1992) in collaboration with S. Teitel (Rochester University, NY) concerns the 3D XY-model of a strongly type-II superconductor. For many years, he has been working exclusively on the classical thermodynamics of vortices in the presence of disorder, using Monte Carlo simulations. His future activities will concentrate on the influence of strong disorder on the vortex lattice and vortex glass transitions. Olsson appears to be working without any collaborators in Sweden, and has not had any external funding since 2001. He also seems to have focused for a long time on a relatively narrow cluster of subjects, using a single method, and he has published a relatively small number of papers. The Expert Panel supports his process of building up a new group at Umeå University.

The Umeå/NORDITA group headed by Petter Minnhagen is rather difficult to evaluate due to a number of rapid changes in its numbers, activities, and physical location. The research activities of the senior member Minnhagen, at Umeå University until 2002, were mainly directed towards classical critical phenomena, especially in vortex systems. Together with an experimental group at Uppsala University, his group found that the 2D – 3D crossover for the phase transition of layered superconductors is also present in bulk YBCO. Part of the activity was also devoted to simulations of models related to Josephson junction arrays and HTSC. The group's future research seems no longer to be connected to superconductors and is more directed towards the field of general network theory. Overall, the work in superconductivity was very good.

### Experimental Activities

The research within Lars Börjesson's group of Condensed Matter Physics (CTH) is divided into four main parts: i) soft condensed matter and disordered materials; ii) strongly correlated materials; iii) energy-related materials; and iv) biological applications of nano-optics. The experimental investigation of high- $T_c$  superconductors (a subject in part ii) addresses issues such as the relation between the normal state and superconducting

properties, and the role of various structural elements (CuO planes, charge buffer layers, etc.) for the physical properties. They investigate the excitation spectrum in a wide energy range using optical techniques. Complementary structural determinations are done using neutron diffraction and computer simulations. The group has a solid track record of fundamental studies in soft matter, and plans to continue its activities in complex oxide materials in a collaborative effort between experimental and theoretical physicists, chemists, materials scientists, etc. They are careful in their choice of systems, and with respect to their published work and the proposed future work, the group has an excellent scientific activity.

The group headed by Eva Olsson of Microscopy and Microanalysis (CTH) includes more activities outside the scope of this evaluation, which was not reported. The research activity in superconductors is directed towards electron microscopy-based studies of grain boundaries and interfaces, which is of great importance for the understanding of the properties of HTSC and other perovskite structures. The work on artificial grain boundaries in thin films provides crucial information on how the structure could be tailored and optimised. They have also been strongly involved (especially Håkan Olin, who left the group) in the combined TEM-STM holder, developed at Chalmers. In the near future, new electron microscopy instrumentation, which allows for 3D-tomography, will be installed (funded by the Wallenberg Foundation). The available electron microscopes of the group are extensive and very important in the study of nanostructures, interfaces, clusters, etc. They also have a strong collaboration with theoretical groups at CTH, performing DFT calculations in order to understand the electronic properties of the group's experimental system. Keeping up with the research forefront based on TEM studies requires, besides expensive equipment, also personnel. Appropriate funding by the Research Council is clearly important for this excellent group.

The Quantum Device Physics group at CTH is divided in three subgroups, all performing research in low and/or high- $T_c$  superconductors. The QuOx subgroup (Tord Claeson and Dag Winkler) has its origin in superconducting electronics and has moved towards oxide-based materials. Present activities include thin film growth and Josephson junction fabrication for devices with quantum limited sensitivity, thin film preparation for SET in HTSC islands, d-symmetry studies,  $\pi$ -junctions, and qubits. The second EMP subgroup (Per Delsing) has a history of doing Coulomb blockade and single-electron physics in small tunnel junctions. They have studied a wide range of systems ranging from single junctions, SET transistors, 1D- and 2D-arrays of junctions, etc. In the framework of quantum computing, Delsing studied the single Cooper-pair box, which

can act as a charge qubit. The Bolometer subgroup (Leonid Kuzmin) activity is directed to the development of supersensitive bolometers, using superconductor-insulator-normal metal (SIN) tunnel junctions. The future plans of the three subgroups are related to some of the most exciting research topics in superconductivity. These activities will deal with the production of thin films in various heterostructures, the realisation of d-wave qubits and HTSC single-electron transistors, the development of RF-SET and high-frequency techniques for application on qubits, the further development of the scanning SET, a super sensitive Josephson spectrometer, etc. The proposed research subjects are challenging and innovative and rely on the development of novel nanometre devices that are of interest both in basic science and for applications. They have already made first-class achievements on such subjects as SET-based qubits, scanning-probe SET's, molecular SET's, etc. This outstanding group has the necessary experience and expertise to achieve substantial breakthroughs in the field of superconducting electronics.

The Condensed Matter Physics group at KTH, headed by Alexander Grishin, consists of two subgroups, one led by Grishin (collaborators: Sergey Khartsev and Sören Kahl) and the other, mainly active in high-temperature superconductivity, is led by Magnus Andersson (Ph.D. in 1992) and Östen Rapp. The work on HTSC can be divided into studies of vortex dynamics, superconducting fluctuations, and electronic transport properties of alloys produced by selective doping. A generalised approach to the vortex glass transition was recently studied, while a vertical vortex solid-to-liquid transition has been found in underdoped YBCO single crystals. Novel flux transformer geometry has been explored and superconducting fluctuations above  $T_c$  have been studied. The future activities, in collaboration with researchers from Palaiseau (France) and Theoretical Physics at KTH, are centred on the vortex dynamics of heavily underdoped YBCO crystals. The planned HTSC activities seem to be concentrated on rather classical subjects, using standard techniques. The overall impression of this subgroup is very good.

Mamoun Muhammed and co-workers within the Materials Chemistry group at KTH are studying a very large and diverse number of subjects. The activities in superconductivity are very good, but limited in scope and related to the development of methods to synthesise nanostructured materials. An interesting and challenging project is the fabrication of HTSC materials with many components, an exact composition, and a high homogeneity, in order to obtain a pure superconducting phase. In collaboration with Argonne National Laboratory and other groups, they succeeded in the fabrication of wires with highly aligned nanoparticles demonstrating

exceptionally high critical current densities. Although in the future planning no superconductivity activities are foreseen, the development of new synthesis methods and tools to fabricate multi-functional nanoparticles will probably be used in the HTSC-context.

Materials Physics, headed by Ulf Karlsson at KTH, has quite a wide range of activities, which include oxide superconductors. The group is a major user of photoemission at MAX-lab and has been responsible for the development of a beamline, which is available to the Swedish user community. The superconducting research is carried out by Oscar Tjénberg (Ph.D. in 1997), who holds one of the Research Council's special research positions. He applies low-energy angle-resolved photoemission (ARPES) to study high- $T_c$  superconductors, demonstrating that the bulk properties of the NdCeO-CuO compound are different from what has previously been thought. Applying the technique of spin-resolved resonant photoelectron spectroscopy, he demonstrated the existence of the Zhang-Rice singlet in several HSTC. In the future, the high-resolution ARPES beamline at Max-lab will permit extremely detailed studies of high- $T_c$  as well as low- $T_c$  superconductors. This is a very interesting approach, which is expected to contribute to the understanding of such systems. Overall, the whole group may benefit from reducing the number of scientific issues to be worked on. The super-conducting activities are of excellent quality.

The Nanostructure Physics group of David Haviland at KTH started in 1997, and established electron beam-based nanoscale patterning technology to form arrays of small Josephson junctions (JJ) operating in the Coulomb blockade, as well as single Cooper-pair transistors (CPT). By using such JJ-arrays and CPT's, the group has obtained important insights into such issues as the coherence of tunnelling and the switching current. They were also able to examine a read-out scheme of charge qubits for quantum computation. Although others pioneered JJ-based charge qubits, this work is important as it addresses one of the fundamental problems to be resolved. The group will continue experiments on phase locking of single Cooper-pair tunnelling, understanding of spin injection into a superconducting strip, and a non-local measurement of spin transport including the effects of gap suppression. This relatively small group has succeeded, in a short period, to build up a first class nanofabrication laboratory and an international reputation in the competitive field of Josephson junction physics. This is an excellent/outstanding group.

The Soft X-ray Physics group at Uppsala University (UU), headed by Joseph Nordgren, has been a worldwide pioneer in the development of soft X-ray emission spectroscopy (SXES) and resonant inelastic X-ray scattering (RIXS) spectroscopy. The group has also used their experimental techniques

to investigate HTSC materials. RIXS offers the unique possibility to study the excitation energies, setting stringent boundaries on important theoretical parameters used for describing these correlated materials. They have shown, for instance, that the 2p-states in the valence band of high- $T_c$  superconducting cuprates pertaining to different oxygen sites could be selectively studied. Their work has resulted in a number of papers in high-impact journals. The group is currently working on making major improvements to the resolution of RIXS, as well as on platforms for *in situ* RIXS studies, which allow variation of temperature and pressure. This dedicated equipment should also benefit the research activities on HTSC. Overall, the group has an excellent reputation, and it has made important contributions to the research community.

The main research activities of the Solid State Physics/Magnetism (UU) group, headed by Per Nordblad, are related to magnetic phenomena. The work in superconductivity is centred on flux dynamics in high- $T_c$  materials. The research in the field of the paramagnetic Meissner effect (PME) has been aimed at searching for manifestations of a glassy low-temperature phase. Certain glassy features including magnetic ageing and rejuvenation phenomena have been established experimentally. Another activity is focused on vortex fluctuations in YBCO and MgB<sub>2</sub> thin films and rests on a close collaboration with Chalmers (Dag Winkler), Umeå University (Petter Minnhagen), as well as with colleagues in Korea and Japan. In the future, they plan to contribute to the understanding of thermally generated vortex – antivortex fluctuations. The group has made important contributions to the Swedish research and remains at the excellent level.

## Future Perspectives

As already discussed in this brief review, due to the complexity of the nature of high- $T_c$  superconductors, there is still much work needed to understand in detail the mechanisms involved in these systems. It seems that to date no theory has been developed, which has predictive power as far as materials systems are concerned. Since purely theoretical approaches so far have difficulties in identifying a clear avenue for search, empirical studies in which materials parameters and properties are correlated with superconducting properties may prove useful. It is important to realise that in this field materials issues are crucial. Microstructures, crystallinity, phase variations, nonequilibrium phases, and the overall structure play an important role and strongly affect the physical properties of the materials. Moreover, it seems that to date there are no clear-cut directions for searches for new superconducting phases, as shown by the serendipitous discovery

of superconductivity in MgB<sub>2</sub>. Research in the electronic properties of high-T<sub>c</sub> superconductors has proved to be particularly fruitful. This has led to improvements in electronic structure techniques, which have an effect on other fields. Mapping the electronic structure with high resolution (in real and reciprocal space) may prove to hold some of the keys to the mechanism of superconductivity. For many applications, electronic or power related, it is important to investigate the mutual interaction between superconductors and other materials. This requires careful preparation and detailed characterisation of inhomogeneous materials, together with measurements as a function of well-defined structural parameters.

*Concerning the Superconducting Activities in the Condensed Matter Physics Community of Sweden, Some General Remarks Can Be Made.*

In the 1991 "International Evaluation of Superconductivity Research in Sweden", 28 research projects of 21 departments or institutes were evaluated in relation to their worldwide activities in this field. The overall balance in the current superconductivity effort, as compared with 1991, is, however, difficult to make since some departments in Chemistry, as well as Materials Science, Metals & Ceramics, and Electronics have not been involved in the current CMP evaluation process.

Of the 16 CMP groups currently active in one way or the other in superconductivity, 14 already had an activity in this field in 1991. Nevertheless, compared with the 1991 situation, there seems to be much less interest and activity in traditional areas, such as bulk synthesis, single crystal growth, structural analysis, electronic structure and spectroscopy, physical properties (T<sub>c</sub>, H<sub>c</sub>, J<sub>c</sub> and flux creep), etc. The current effort in the HTSC high-field, high-current, applications is limited to only one group (Materials Chemistry, KTH).

The overall number of people, the different areas studied, the budget, and the interest has substantially decreased, a phenomenon also visible in other European countries, the USA, and even in Japan. This general trend is influenced by the decreasing level of support for superconductivity from Swedish and European Institutions, as well as from the industry.

Activities in the topical area of "stripe-formation" are limited to numerical work by Stellan Östlund (CTH) and, to a lesser extent, by Krister Karlsson (the University of Skövde). Research on vortex systems is concentrated in the theory groups of Hans Weber (LTH), Jörgen Rammer (UmU), Petter Minnhagen (UmU/Nordita), and the experimental groups of Alexander Grishin (KTH) and Per Nordblad (UU). The synthesis of new materials for practical high-power applications is centred in the group of Mamoun Muhammed (KTH); the effort, however, seems very limited. Ulf Karlson (KTH) and Joseph Nordgren (UU), within the much broader activities

of both groups, perform photoemission and X-ray spectroscopy studies. Finally, Lars Börjesson (CTH) and Eva Olsson (CTH) will continue investigations by optical techniques, neutron diffraction, and TEM. Most of these activities are embedded in a much broader research interest of the groups, and might even be substantially reduced in scope in the future.

The Expert Panel notes, however, that a remarkable and leading role on the world scene is being played by the groups headed by Per Delsing (CTH) and David Haviland (KTH) in the fields of superconducting electronics and qubits for quantum computing purposes. The efforts in thin film, superlattice, and tunnel junction fabrication are clearly very competitive. The theory groups of Vitaly Shumeiko (CTH) and Mats Jonson (CTH) have joined this effort, and they collaborate with different models, in the proposals for new devices.

Overall, the Panel believes that Sweden has an excellent potential to play a significant role in the areas of superconducting nanoelectronics and quantum computing. This programme should be strongly supported and strengthened, and would benefit from an enhanced interaction between the existing experimental groups and other theory groups.

## Condensed Matter Theory

### International Perspective

Condensed matter theory (CMT) is a very broad label, which includes or overlaps with statistical physics (and off-shoot areas, such as network theory, econo-physics, traffic flow, etc), materials theory, optics, and bi-physics. It deals with basic science questions, which are just as fundamental, in their own way, as those addressed by high-energy theorists and cosmologists. However, unlike those fields, it is closely related to inventing and developing new technologies

The fundamental problem for condensed matter theory is to understand the collective behaviour of large numbers of constituent particles (usually electrons and/or atoms). Only systems with very small numbers of particles can be resolved exactly using realistic models. Nonetheless, in many situations macroscopic objects containing around  $10^{23}$  particles are rather well understood. This is due to simplifications that arise from large numbers, as the founders of statistical physics discovered.

A major theme for CMT has been “emergent phenomena”, which exemplify P.W. Anderson’s credo “more is different”. Certain types of behaviour can arise from the interactions between large numbers of particles that do

not occur for small numbers. A famous example of this is “spontaneously broken symmetry”. The spin of an isolated atom will fluctuate thermally and quantum mechanically between different directions (in the absence of any field preferring a particular direction). However, a macroscopic number of spins, due to their mutual interactions, may spontaneously choose to order in a particular direction leading to ferromagnetism and related phenomena. The concept of spontaneous symmetry breaking, first developed in the condensed matter context, later played a very important role in high-energy theory. Other important emergent phenomena involve various types of quasi-particles. These include exciton, magnons, and Cooper pairs. More recently, the fractional Hall effect dramatically demonstrated that quasi-particles can sometimes carry quantum numbers that are fractions of those of the underlying constituents.

A large part of condensed matter theory is concerned with the electronic structure of the ground state and the energy bands of various solids. This area is often associated with the name Density Functional Theory (DFT). In the standard (Kohn-Sham) formulation, it is based on calculating the eigenstates (energy bands) of a single electron moving in an effective periodic potential produced by the ions and electrons. Despite the fact that electron – electron interactions are usually only treated approximately in this approach (for instance in the local density approximation), remarkable agreement with experimental data is often obtained for ground state properties. However, this approach is often inadequate for calculating excited state properties, bandgaps and properties of quasi-particles like phonons and magnons. Furthermore, it is known to fail for some strongly correlated materials like high- $T_c$  superconductors. At least in some situations, partial justification for such a simple treatment of electron – electron interactions can be found in Landau’s Fermi liquid theory.

Increasingly refined DFT techniques and codes have been developed over the years, which require large amounts of computer power to analyse complex solids, solid surfaces, and other systems of reduced dimensionality. The search for better materials for technological applications provides powerful motivation to apply DFT to an ever-growing list of compounds. An important recent application of DFT is in the study of the electronic structure of nanostructured materials. The lack of periodicity in such systems places additional demands on DFT codes and emphasises the need for innovative computational techniques for realistic simulations of these systems. The expected technological applications of nanoscale materials, aided by several recent initiatives sponsored by funding agencies worldwide in creating materials by design, have sparked intense activity in the area. DFT calculations are playing an important role in research projects, which

aim at the development of theoretical and computational frameworks for accurate and reliable understanding of nanoscale material. DFT calculations are also serving as the building blocks for the highly attractive field of multi-scale modelling, whose importance in designing (and hence controlling properties) of novel materials is not to be denied. Another emerging area in which DFT calculations are expected to provide critical input is in the understanding of biological systems.

A further field of CMT, which seems to have developed a distinct identity in the last fifteen years or so, sometimes goes under the name of “strongly correlated electrons”, or more generally “strong correlation physics”. Two developments in the 1980’s gave this field a huge lift. One of them was the amazing experimental discovery of the fractional quantum Hall effect in very clean two-dimensional electron gases in high fields, quickly followed by its theoretical explanation by Laughlin. The other one was the experimental discovery of high- $T_c$  superconductivity in copper-oxide materials.

Further elucidation of the fractional Hall effect has been a major international theoretical success story of the last 20 years. This includes understanding the various filling fractions at which conductance plateaux take place, which require quite ingenious generalisations of Laughlin’s theory of the  $1/3$  plateau, understanding the role of edge states, treatment of double-layer Hall systems, and study of tunnelling phenomena at constrictions and edges of Hall bars.

The high- $T_c$  discovery sparked an enormous international theoretical response that, so far, has not led to any widely accepted explanation of the phenomenon. The high- $T_c$  oxides are not at all conventional metals at higher temperatures, but are two-dimensional lightly doped “Mott-Hubbard insulators”. A straightforward application of band theory would predict that the undoped parent compounds are metals. In reality, they are insulators due to the crucial effects of electron – electron interactions. A theory of lightly doped Mott-Hubbard insulators has become a holy grail for CMT. The high- $T_c$  field is at once important from the applications’ viewpoint and very exciting for the basic physics issues that it raises.

The enormous attention paid to high- $T_c$  superconductivity has heightened interest in several related fields, including low dimensional magnetism, non-Fermi liquids, such as the Luttinger liquid (which occurs in one dimension), and quantum phase transitions. The development of nanoelectronics and the search for solid-state qubits have also stimulated activity in the strong correlations field, such as the occurrence of the Kondo effect (including its multi-channel versions) in quantum dots. The young field of quantum computing and information has led to general work on quantum coherence, and ideas such as “quantum computing with anyons”, which borrows ideas

from the strong correlations field. The exciting experimental progress in trapping of cold atoms in optical lattices has provided further impetus to the theory of strongly correlated systems. Trapped fermionic atoms might be accurately described by the same (Hubbard) model that is commonly used as a greatly simplified approximate model for the electrons in high- $T_c$  superconductors, and may provide crucial insight into the behaviour of the Hubbard model, and hence into the high- $T_c$  superconductivity puzzle. Among theoretical methods that are applied to strongly correlated materials, an increasingly important role is played by numerical techniques: exact diagonalisation, quantum Monte Carlo, and Density Matrix Renormalisation Group.

One interesting development of the last decade on the international scene has been a coming together of theorists working on DFT and strongly correlated electrons via the development of “Dynamical Mean Field Theory”, based on the infinite-dimension limit of interacting tight-binding models. Work in this area has dealt with such fundamental issues as the Mott-Hubbard transition; and also, more recently, with trying to fit the detailed band structure of complicated materials.

Another distinguishing feature in CMT in the past three decades has been an emphasis on understanding phenomena at solid surfaces and interfaces. Apart from expected technological applications, the reduced periodic symmetry and presence of regions of varying co-ordination make surfaces and interfaces interesting grounds for the formulation of theoretical concepts. Tremendous advances in experimental techniques over the past three decades have made it possible to isolate surface effects from phenomena in bulk solids. Theorists have responded with a multitude of theoretical and computational methods to explain novel behaviour of solid surfaces, and provided insights into the dependence of system properties on local structure and dynamics. The ability to predict and control the nature of the interaction between atoms and molecules on solid surfaces and at interfaces has helped foster a strong link between condensed matter physics and surface and materials science. In fact, a large part of condensed matter theory is directed towards understanding and designing novel and functional materials with interesting surface properties.

Of course, there are many other active fields of CMT besides DFT and strongly correlated systems. Notably, these include the study of quenched disorder (including glasses) in both classical and quantum contexts, soft surfaces and biologically inspired theory including protein folding, mechanical properties and phase transitions of surfaces, thin film growth, etc. Some theorists with a background in statistical physics are also venturing into fields such as economics, traffic flow, and general theory of networks.

## Condensed Matter Theory in Sweden

Here, we attempt to divide theoretical condensed matter activities in Sweden into a number of subfields: electronic structure (both bulk and surface), transport and nanoscale physics, strongly correlated systems, classical statistical physics and biophysics, and other areas. Note that we here choose to classify theoretical research by its physical applications rather than its theoretical methodology (DFT, Monte Carlo, field theory, etc.). Much of the work mentioned below is also discussed in the descriptions of the other specific scientific areas.

### *Electronic Structure (Bulk and Surface)*

This is by far the largest, best funded, and most successful subfield of CMT in Sweden. It has a long and illustrious history in Sweden, going back at least to Stig Lundqvist and Lars Hedin in the 1960's, followed by seminal work by Bengt Lundqvist and Börje Johansson in the 1970's. In fact, these individuals and their outstanding achievements have helped to make Sweden one of the Meccas for theoretical and computational studies of materials and surface physics.

For a long time, much of this work has been, and it continues to be, based on DFT. Some of the influential current work involves extending the DFT formalism in various ways, as in the case of Per Hyldgaard and Bengt Lundqvist (Materials and Surface Theory group at CTH) who are extending DFT to include van der Waals interactions. They have also refined DFT for applications to out-of-equilibrium transport and dynamics. Several advancements to DFT computational codes are being developed in Sweden, notably by Shiwu Gao at CTH, Rajeev Ahuja (Condensed Matter Theory, UU), and also by Olle Eriksson and others within the Theoretical Magnetism group at UU. Furthermore, Igor Abrikosov (Theory and Modelling, LiU) and Krister Karlsson (the University of Skövde) are involved in combining DFT with Dynamical Mean Field Theory. Additionally, Elsebeth Schröder, in Lundqvist's group at Chalmers, has developed an efficient DFT-van der Waals method for the direct evaluation of crystalline structure, bulk modulus, and bulk-modulus pressure derivative of novel surface-oxides.

Eriksson's group (UU) is engaged in applications of DFT to magnetic systems. This includes the calculation of anisotropy parameters of magnetic materials, including magnetic multi-layers and nanostructured materials, and the study of non-collinear magnetic order. The excellent work of Lars Nordström (in Eriksson's group) in the area, has led to the predictions of magnetic anisotropy energies and identification of a FeCo alloy with very high such energy. This work has applications to giant magnetoresistance and

spintronics areas, in which the group works closely with experimentalists, as well as with partners in industry.

Another example of excellent applications of DFT to magnetism (which led to a cover picture in *Nature*) involving Igor Abrikosov (now at Theory and Modelling, LiU) and Börje Johansson (Condensed Matter Theory, UU), concerned the INVAR effect (the absence of thermal expansion in specific magnetic alloys). Abrikosov is now promoting further research in understanding the electronic structure of magnetic materials, which is carried out in his new position at LiU, where he is heading a large, active, and diverse group in theory and modelling.

Börje Johansson's group at Uppsala University has pioneered work in understanding and predicting structural stability, phase transitions, electronic and, in some cases, magnetic properties of advanced materials, such as transition metal oxides, ternary alloys and their complexes, and transplutonium metals. The natural inclusion of the effects of high pressure and temperature on a number of metals and alloys has added a broader appeal to the outstanding/excellent work of this productive group.

The Materials and Surface Theory group at Chalmers (headed by Bengt Lundqvist), with the goal of comprehending and predicting the properties of solid surfaces, is performing internationally leading work. This group too, works very closely with experimentalists, both in-house and elsewhere. Such synergistic activities between Bengt Lundqvist, Stig Anderson, and Bengt Kasemo have placed Chalmers high on the world map of surface physics. More recently, Mats Persson (Materials- and Surface-Theory, CTH/GU) has been working closely with the experimental STM group of Wilson Ho, at the University of California (Irvine), on the manipulation and characterisation of matter at the nanoscale. The tradition is also being upheld by Göran Wahnström, Per Hyldgaard, and Shiwu Gao, each of whom engages in collaborative research with leading experimentalists worldwide. Outstanding theoretical work by Göran Wahnström and co-workers, in Bengt Lundqvist's group at CTH on diffusion at solid surfaces, straddles the quantum and classical treatments of the subject and provides measures for isolating them. Their development of coupled techniques, capable of treating phenomena on different time and length scales, has led to a better understanding of the dynamics of molecular dissociation at metal surfaces. Shiwu Gao's theoretical formulation of dissipative quantum dynamics at surfaces, is a significant contribution since it addresses the important role of friction, inelastic tunnelling, vibrational damping, and other mechanisms for energy transfer in determining the branching ratios of competing chemical reactions of adsorbates at surfaces. At the same time, Per Hyldgaard's recent excellent DFT-based work on substrate-mediated

interactions has been critical to the understanding of experimental observations in epitaxial growth on Cu and Ag surfaces.

Some excellent surface electronic structure calculations are also being carried out within experimental groups in order to analyse their experimental data, notably in the Quantum Chemistry group of Anders Nilsson at SU, whose members are applying DFT to analyse their experiments on chemical bonding of adsorbates at surfaces. Börje Johansson's groups (at UU and KTH) have successfully explored the possibilities of DFT and related methods, by applying them to metals under high pressure and temperature, including the earth's mantle, resulting in publications in prestigious journals. The applied orientation of these two groups has also taken on the task of studying stainless steel and materials for the storage of nuclear waste. Bo Helsing in Lars Walldén's group (Solid State Physics) at CTH/GU is carrying out very good theoretical calculations to explain surface phenomena, such as the effect of alkali addition on the lifetime of surface electronic states, which is studied experimentally by the group.

### *Transport and Nanoscale Physics*

Many groups are studying transport from a variety of viewpoints. Furthermore, many CMT groups in Sweden, following the trend worldwide, have recently become involved in various aspects of nanophysics. Several groups are studying transport through nanostructures such as quantum dots.

At Chalmers University of Technology (CTH), the Condensed Matter Theory group of Mats Jonson proposed an interesting "shuttle" mechanism for charge transport through Coulomb blockaded nanostructures. This work has resulted in several publications in prestigious journals and, furthermore, a patent – an internationally competitive research contribution. Vitaly Shumeiko and Göran Wendin (Applied Quantum Physics at CTH) have been doing noteworthy work on superconducting qubit candidates for a future quantum computer. One interesting project involves a readout mechanism for a "Cooper-pair box"-type qubit, based on coupling this qubit to a single-electron transistor (i.e., another quantum dot in the Coulomb blockade regime containing an odd number of electrons). They have also proposed another type of superconducting qubit involving an Andreev bound-state localised near a quantum point contact. This is an important contribution to this rapidly developing and exciting field.

Mats Persson's (Material and Surface Theory at CTH/GU) strong collaborations with some of the leading experimental groups in STM has provided a fundamental understanding of vibrational inelastic electron tunnelling in STM junctions, which we regard to be internationally leading condensed matter physics research. Carlo Canali (Kalmar University) is making a

promising contribution within theoretical nanoscience, studying tunnelling through ferromagnetic nanoparticles.

Further very good work within this area (of which some are also mentioned in other sections above) includes: Carl-Olof Almladh and Ulf von Barth (Solid State Theory, LU) on development of the theory of time-dependent DFT to study conductivity of solids; Karl-Frederik Berggren (Theory and Modelling, LiU) and Igor Zozoulenko (Mesoscopic Physics and Nanoelectronics, Campus Norrköping) on transport through quantum dots with chaotic spectra, using semi-classical methods; Sergei Simak (who recently moved to LiU) on transport through gold nanowires; Olle Eriksson and others (Theoretical Magnetism, UU) studying transport through a Coulomb-blockaded quantum dot using approximate Green's function methods; Koung-An Chao (Solid State Theory, LU) on thermal transport in low dimensional systems; Sven Stafström *et al.* (Theory and Modelling, LiU) on transport through conjugated carbon systems, including DNA; Jörgen Rammer and Andei Shelankov (Theoretical Physics, UmU) developing a novel approach, based on counting statistics, for analysing charge transport through nanostructures.

Good work is also performed by Ulf Ekenberg (Photonics and Microwave Engineering, KTH) studying the Data-Das transistor and the Rashba effect, which involve spin-orbit effects in the transmission of electrons through a semi-conductor channel.

### ***Strong Correlation Physics***

Strong correlation physics is a major focus of the Solid State Theory group (Stellan Östlund, Hendrik Johannesson, and Mats Granath) at CTH/GU, the Condensed Matter Theory group (Anders Rosengren, Patrik Henelius, and Mats Wallin) at KTH, and the Fields and Particle group (Hans Hansson and Anders Karlhede) at SU. The researchers in these groups cover a wide spectrum of approaches to the enigmas of this area, briefly touched upon in the following paragraph. Stellan Östlund, Hans Hansson, and Anders Karlhede are engaged in excellent/very good work on an unusual, innovative, higher spin, version of the Hubbard model that seems amenable to a novel type of approximate solution, which may turn out to be highly accurate. In another very good effort, Hendrik Johannesson applies the Bethe ansatz, and bosonisation techniques, to the study of quantum impurity models (Kondo, Anderson, etc.) and Luttinger liquids. Mats Granath is also carrying out very good work on stripe phases in high- $T_c$  superconductors, in collaboration with S. Kivelson, one of the dominant theorists in this field. Anders Rosengren has been doing excellent work on random quantum spin chains and Kondo lattice models. Very good work by Patrik Henelius focuses

largely on random quantum antiferromagnets, using two powerful numerical methods: density matrix renormalisation group and quantum Monte Carlo. The very good work of Mats Wallin is on quantum bosons in optical lattices. Finally, a very good effort of Anders Karlhede in strong correlation physics has recently been directed to the quantum Hall effect with a half-filled Landau level. Some other groups, whose main focus is elsewhere, have also worked in the strong correlations field: good work of Michael Lieberman (Condensed Matter Theory, UU) is currently centred on exciton superconductivity, and an excellent effort of Bengt Lundqvist (Materials and Surface Theory, CTH), based on DFT, led to the prediction of a new and highly ideal one-dimensional electron gas system that would form on a low-symmetry oxide surface. This system could be useful for studying strong correlation physics (Luttinger liquid behaviour). The excellent effort by Igor Abrikosov (Theory and Modelling, LiU) and Krister Karlsson (University of Skövde) in combining DFT with Dynamical Mean Field Theory appears to be promising. The Panel also noted the very good work of Jari Kinaret (Condensed Matter Theory at CTH, along with group leaders Mats Jonson and Robert Shekhter) on Luttinger liquids.

In Lund, Stephanie Reimann (Mathematical Physics) works on the ground state properties of electrons in ideal quantum dots, and arrays of quantum dots, and the related problem of cold atoms in optical lattices. The methods used are exact diagonalisation, configuration interaction, and density functional theory. This relatively young researcher (Ph.D. in 1995) is maintaining vigorous international collaborations, publishing her work frequently in prestigious journals, and bringing new methods and research topics to Lund, and Sweden in general: a promising new initiative, which should be encouraged.

### *Classical Statistical Physics, Biophysics, and Related Topics*

Kim Sneppen at NORDITA is a well-known theorist with many highly cited papers in prestigious journals that cover a number of topics including models of evolution and protein networks. Although he has never worked for an extended period in Sweden, as far as we know, he is currently being funded by the Swedish Research Council to do research in Copenhagen. If he eventually moves to Sweden, could this be a major gain for Swedish CMT. Mats Wallin and Jack Lidmar (Condensed Matter Theory, KTH) are versatile and relatively young (Ph.D. in 1990/1997, respectively) theorists working on a number of interesting and multi-disciplinary projects, using a partly numerical approach. These projects include disordered vortex lines in superconductors, and very recent work on molecular motors (by Mats Wallin *et al.* at the Karolinska

Institute) and on buckling of viruses (by Jack Lidmar with D. Nelson at Harvard).

Further very good work within this area is being performed by: Mikhail Dzugutov (KTH) on fundamental properties of liquids and amorphous solids using molecular dynamics simulations of pairwise interactions; Bernhard Mehlig (Solid State Theory, CTH) on a stochastic approach to understand the decorrelation of gene histories along the human genome; Lennart Sjögren (Solid State Theory, CTH) on glassy dynamics; Thomas Guhr (Mathematical Physics, LU) on classical chaos; Peter Olsson (Theoretical Physics, UmU), Petter Minnhagen (NORDITA-UmU), and Hans Weber (Division of Physics, LuTH) on classical phase transitions involving vortex lattices in superconductors. Weber (UmU) has also started working on statistical models of traffic flow, and Petter Minnhagen, currently director of NORDITA, has recently diverted his research activities to general theory of networks, in collaboration with Kim Sneppen.

### *Other Activities*

Very good/excellent work is also performed in the Theory and Modelling group at Linköping University (LiU). Bo Sernelius works on Casimir and van der Waals forces between real metal plates, as well as on surface modes in physics. He has become well known to the public because of his research into the effect on humans of the radiation from cellular phones, which may lead to attractive forces between blood cells. Peter Münger's work on cluster diffusion using MD and DFT led to the prediction of reptation mode (snake-like) of diffusion of Pt heptamers on Pt(111). Joint work with an experimental group at LiU verified his theoretical model.

Anders Rosengren (Condensed Matter Theory, KTH) has worked on impurities in D-wave superconductors (highly cited work from over ten years ago with Altshuler and Balatsky, well-known U.S.-based theorists). In addition, Mikael Fogelström (working in the Applied Quantum Physics group, CTH) has done highly cited work on tunnelling into D-wave superconductors, while he was working with Sauls at Northwestern University, in the USA.

Furthermore, Thomas Guhr (Mathematical Physics, LU) has carried out very good collaborative work with experimentalists on a study of the acoustic resonances of aluminium blocks, showing that they obey either Poisson or Gaussian orthogonal ensemble statistics depending on the block shape. He wishes to extend his research to the study of mechanical properties of nanostructures.

Peter Johansson (Solid State Physics, UmU) and Peter Apell (Condensed Matter Theory, CTH) conduct very good theoretical calculations of the

electromagnetic response of nanometre-sized systems by solving classical equations in complex geometries. Non-linear dynamical lattice models are studied by Magnus Johansson (Theory and Modelling, LiU). Rolf Riklund, in the same group, has been involved in excellent calculations of non-linear phenomena for anharmonic lattices. Excellent work has been conducted in the group of Sven Stafström (Theory and Modelling, LiU), who has been engaged in examinations of lattice and electron dynamics and their application to explain phenomena as varied as charge transfer in solar cells, electrical conduction (or lack of) in DNA, polaron dynamics in polymer chains, and charge separation in fullerenes.

### *General Remarks on Condensed Matter Theory in Sweden*

From the data provided by the Research Council to the Expert Panel, it seems that about 22 out of 63 CMT grant holders (35%) do work largely based on DFT, and that they received 47% of the Research Council-CMT funding, over the last four years. They supervise roughly half of all theoretical Ph.D. students and post-docs. This research is mentioned above under “Electronic Structure” and a part of it can also be found under “Transport and Nanoscale Physics” and “Other”. These numbers may largely reflect the remarkable influence of two very distinguished senior theorists: Börje Johansson and Bengt Lundqvist. DFT-related research seems unquestionably to be the strongest field of CMT in Sweden, as it has been for many years. Together with their co-workers and fellow experimentalists, they have pioneered many advances in the applications of DFT in order to explain surface and materials properties, and given Sweden a leading edge in the two areas. This is a remarkable achievement for a country as small as Sweden. Consequently, the percentages of researchers and funding in DFT-related areas are considerably higher than in other countries. This disparity has, of course, led to a division between the haves and the have-nots, and hampered the morale in several places, as was seen in the written and verbal comments made by the individuals to the Expert Panel.

On the other hand, only about 9 out of 63 grant holders work primarily on strongly correlated physics, and they are generally much more poorly funded and have far fewer Ph.D. students and post-docs per capita. Some fields, which are very popular in other countries, are barely represented at all in Sweden. Researchers in Sweden appear to have had little impact over the last 15 – 20 years on the theory of the quantum Hall effect, or on fundamental theories of high- $T_c$  superconductivity and related areas. Exceptions to this statement are some highly cited work on vortices and on Density Matrix Renormalisation Group, which was done in Sweden about 10 years ago. Furthermore, some researchers in Sweden made major contributions to

these fields when they were working outside Sweden earlier in their careers, over a decade ago. There is only a small amount of theoretical work on quantum-disordered ground states of antiferromagnets, Kondo lattices, or quantum bosons and fermions in optical lattices.

At the same time, there is a relatively small amount of *experimental* work going on in Sweden in strongly correlated physics areas, such as the quantum Hall effect, *fundamental* research into superconductivity (as opposed to more applied research involving junctions), pressure or chemical substitution induced quantum phase transitions in heavy fermion systems, studies of magnetic systems with unconventional ground states, inelastic magnetic neutron scattering, studies of quasi-one-dimensional organic conductors, and work on cold atoms in optical lattices. It is a bit hard to say whether the small experimental effort in these areas has led to the small theoretical effort or vice versa. The few theorists working on strongly correlated systems in Sweden generally do not appear to have good contacts with experimentalists.

Theoretical biophysics also seems under-represented within the condensed matter physics community in Sweden. (This is especially true if we do not include Sneppen, who apparently has not actually worked in Sweden yet.)

Several theorists mentioned the lack of communication and collaboration between different groups in Sweden. Motivated by funding opportunities, some of these theory groups are aggressively forming collaborations elsewhere in Europe. Ironically, in many cases, we were left with the impression that they are not talking as much as they should to the theorists in competing groups in their own university or across the country. One possible cause of this lack of communication is the present funding problems associated with university positions, described at the beginning of this document, which are contributing to a bunker mentality and unhealthy competitiveness between different groups. Lack of communication between different theory groups may in the long run weaken the overall research effort in condensed matter theory, since it is often useful to tackle the same problem using more than one method. It may also weaken the education of graduate students, since they miss the opportunity of being exposed to a larger set of approaches to physics. One example of a missed opportunity may be Dynamical Mean Field Theory, mentioned above. This might have led to collaboration between researchers in Sweden from the DFT and strongly correlated electrons communities, but has not done so yet. (There is a minor effort in Sweden in this overlap area, coming entirely from the DFT side, as mentioned above. The strongly correlated side is coming from outside Sweden.)

Some theoretical research activities in CMP require strongly concerted efforts of a number of theorists to solve some complex and computationally

challenging problems, while other areas in the field are better served through research activities conducted by small groups with size down to one senior researcher. The ideal system should have the flexibility of allowing and rewarding both group and individual efforts. The main advantage of such a structure would be to encourage broader diversity in research in condensed matter theory. The lack of diversity in research opportunities and the pressure to be associated with larger groups were complaints that the Panel heard at several places. To ensure high-quality research activities irrespective of group size, the Expert Panel *recommends* funding to be based on quality of the proposed work irrespective of whether the group is large or small. Clear policies on this point may also help remove some of the internal competition for funds and prestige. It may also bring in more diversity in research areas.

Another issue brought up by many grant-holders, both theorists and experimentalists, concerned the perceived pressure to do applied research. One researcher commented: "This often leads to pseudo-applied research, which is neither good for the theoretical progress nor the technical progress". The general problem of funding university positions and the resulting climate of fear tends to make researchers work in "safe" areas, where they think funding is more likely because of possible applications of the research. Some researchers commented that they would send their more original and risky research proposals to the SSF, rather than to the Research Council. This is ironic, since the Research Council is supposed to be funding basic research, while the SSF is supposed to be funding applied research. This pressure to do applied research probably plays some role in the dominance of DFT-related condensed matter theory research in Sweden. DFT is a powerful tool for investigating detailed properties of materials of possible technological relevance. Other fields of CMT are more focused on general principles and offer far less immediate prospects for applications. These run the risk of being stifled by the pressure to do applied research. This leads the Expert Panel to encourage the Research Council to adhere to its mandate to support basic research.

## Future Perspectives

It would be foolhardy for us to make detailed predictions about what areas of CMT will be important in the future. This can change overnight with new experimental discoveries or a new theoretical breakthrough, as was illustrated by the fractional quantum Hall effect and high- $T_c$  superconductivity. Theorists, not requiring experimental equipment, are able to change fields very rapidly, in response to new developments. Nonetheless, we venture to offer some comments.

One trend, which does seem clear, is the increasing importance of computational techniques, due largely to the impressive computer speed-up in recent decades and important algorithm developments. Certain models, which were only partially understood a decade or two ago, are now solved in remarkable detail numerically. Unless computer speed-up and algorithm breakthroughs abruptly end, this increasing importance of computational techniques seems destined to continue.

As is true in other parts of the world, a good number of condensed matter theorists in Sweden are turning to theory and modelling of nanomaterials, as well as pursuing the trendy area of multi-scale modelling of materials. This is a positive trend and should be encouraged.

Efforts to combine the detailed *ab initio* approach of DFT with methods for tackling strongly correlated systems, such as Dynamical Mean Field Theory, seem likely to be of increasing importance, and is perhaps a natural field for Sweden.

The relentless push to apply methods from CMT to other fields, such as biophysics, economics, traffic flow, etc., also seems likely to continue. It is usually very difficult for people entering a field from an unusual background to make contributions that are instantly accepted or appreciated in that field. Nonetheless, this cross-fertilisation occasionally leads to great breakthroughs, and should be encouraged.

## Soft Condensed Matter, Biophysics, and Biomolecular Materials

### International perspective

Within the last two decades, soft condensed matter has emerged worldwide as a highly active subfield of condensed matter physics. This multi-disciplinary field explores the physics of a range of materials, which are of interest both in applications and in understanding of fundamentally new physics concepts. Soft matter refers to partially ordered (e.g., liquid crystalline matter) or disordered phases, where the constituent molecules or macromolecules have organised on large length scales, typically between nanometres to microns. Soft matter systems exhibit new dynamics associated with their thermally activated collective modes that are substantially slower as compared to dynamics (rotation, diffusion) in simple liquids. Among the most actively studied systems worldwide are liquid crystals, surfactant solutions of micelles and microemulsions, colloidal suspensions, and

polymers. Soft matter research and development has already had a major technological impact worldwide, for example, in the multi-billion-dollar plastics (e.g., used in automobile parts, toys, and other chemical products) and liquid crystal display industries, and in the petroleum and cosmetics (creams and gels) industries.

Research in biophysics over the last four to five decades has primarily centred on studies of the structure and phase behaviour of biological lipid membranes. Even to this date, the vast majority of biophysical studies of membranes have been on rather simple model membrane systems consisting of one or a few types of lipid mixtures, which contain a low concentration of protein inclusions. In these systems, relatively simple questions are addressed. For example, there are groups that investigate the interactions between membranes to test theoretical ideas regarding surface forces. Many groups investigate either the effect of membrane elasticity on the long-range interactions between proteins, or the renormalisation of the bare elastic moduli of the membrane due to the proteins. Membranes of living organisms are complex structures with the lipid bilayer, containing membrane proteins and protruding carbohydrate chains, which are involved in many biological functions including cell-cell recognition and cell-signalling, energy transduction, and the generation of the action potential to enable nerve cell communication. An important current challenge in biophysics research is in the development of new techniques, which would allow *in vitro* studies of real biological membranes.

More recently, over the last one or two decades, the international biophysics community has also turned their attention to studies of proteins (the molecules that are responsible for the vast majority of cellular activity and do most of the work in organisms on many length scales from nanometres to many microns). One group has devoted itself to single-molecule studies, which include, for example, the elucidation of force generating capabilities of single motor proteins, the precise method by which motor proteins walk on their biological tracks, the molecular motors responsible for the packaging of entire viral genomes into the viral capsids (a protective outer shell), and the nanoscale mechanical properties of filamentous proteins, to name a few areas. The other group of researchers is involved in studies of supramolecular biophysics, where the collective properties of proteins are explored. The physical concepts involved often have analogies with concepts developed in the context of soft condensed matter physics.

At present, numerous laboratories worldwide are focused on understanding collective interactions between proteins, which in turn lead to a variety of supramolecular hierarchical structures, spanning lengths from Ångströms to the micrometers. The ultimate goal of many such studies is to relate the

structure to a particular cellular function. Biophysicists have been studying the mechanical and structural properties of filamentous (F)-actin (one of the three components of the cytoskeleton, the skeleton of eukaryotic cells) for more than a decade. F-actin further assembles to form either bundles, or loosely packed 2D and 3D network structures in cells. The distinct functions, resulting from these highly regulated structures interacting with other biomolecules and motors, include cell shape and mechanical stability, cell adhesion and motility, and cell cytokinesis, the physical splitting of a cell into two daughter cells. However, the molecular details of how a specific supramolecular structure enables a specific function remain unknown, and constitute a very active area of research.

A strong motivation for biophysical studies arises from the expectation that the process of learning about the manner in which nature performs work at the very small subcellular scales, should pave the way towards the development of functional miniaturised materials for many future applications. As we describe below, little activity of this nature is currently pursued within condensed matter physics groups in Sweden.

From a fundamental theoretical perspective, the mechanisms leading to supramolecular structures are poorly understood, and remain a very active area of theoretical biophysical research. While we have a better understanding of self-assembly at thermal equilibrium, which occurs, for example, when lipids assemble into membranes; out-of-equilibrium assembly in energy dissipative systems remains poorly understood. Examples of the latter include biological and soft matter systems under flow and biomolecular assembly and disassembly involving hydrolysis of high bond-energy molecules (adenosine triphosphate) ATP or (guanosine triphosphate) GTP. The GTP-dependent assembly and disassembly of microtubules, which is critical to cellular transport and chromosome separation in a dividing cell, is a well-known example, where many fundamental concepts regarding the assembly and disassembly remain to be elucidated.

A rapidly emerging new field, which combines soft condensed matter physics and biophysics, is the field of biomolecular materials. Biomolecular materials are materials that result from research at the interface between physics, chemistry, engineering, and biology. The multi-disciplinary research draws upon workers from soft condensed matter physics, biophysics, chemical synthesis, biochemistry, molecular cell biology, and genetic engineering. A common theme of such materials is self-assembly into hierarchical structures. In many cases, the materials are used in biomedical applications, for example, as drug and gene delivery vehicles. Often biomolecular materials contain functionalised interfaces, where the functionality is derived from biological molecules, which may be manipulated at the

molecular level. For example, a key ingredient of functionalised biomolecular materials that act as biosensors, is immobilised receptor biomolecules that can sense their ligands (the molecules to be sensed) through specific ligand – receptor interactions.

Other biomolecular materials, which have received much attention at the worldwide level, include two-dimensional assemblies of membrane-proteins such as bacteriorhodopsin and surface protein layers. Research in these systems is leading to the development of advanced materials, to be utilised in molecular electronics and as optical switches, and for the lithographic fabrication of nanometre scale patterns.

### **Biomolecular Materials, Biophysics, and Soft Matter in Sweden**

The effort in soft matter and biophysics as part of condensed matter physics in Sweden can be divided into four areas of research. These include biomolecular materials, biophysics, soft matter, and new techniques. However, the boundaries between these research areas are becoming increasingly fuzzy, as multi-disciplinary research becomes more common.

#### ***Biomolecular Materials (Both Medical and Non-Medical Materials)***

Mamoun Muhammed *et al.* at the KTH are involved in excellent materials chemistry research on developing new methods to synthesise nanoparticles and nanostructured materials. The long-term motivation for the research is to make functional materials tailored for applications, for example, in medicine for magnetic resonance imaging, and in targeted drug delivery.

The materials synthesis approach employed by the investigators uses a bottom-up approach and also directed assembly of nanoparticles on patterned surfaces containing specific molecules, which act as receptors and selectively bind the nanoparticles. The group is able to synthesise nanoparticles with controlled morphology, including spheres, rods, and sheets (i.e., referred to as first generation materials). Recent work from the group has been published, where first generation nanoparticles have been functionalised, for example, through surfactant coating of magnetic particles for use as contrast agents for magnetic resonance imaging (second-generation nanoparticles). An ongoing project is the development of drug-carrying particles *in vitro* for the purpose of targeted delivery of drugs *in vivo*. The multi-structured materials consist of a biodegradable polymeric matrix containing temperature-sensitive polymer-drug nanoparticle complexes.

This highly innovative synthesis group has strong ties with international physics characterisation groups, including those at synchrotron radiation (e.g., the photon factory in Japan and the ESRF in Europe) and neutron

facilities, which allow for diffraction structure determination and structure – function studies. The group has a fruitful collaboration with theoretical groups for structure – property predictions.

A promising new multi-disciplinary project led by Hans Siegbahn *et al.* at Uppsala University involves collaboration with biologists and medical doctors from the medical school in developing biocompatible heparin-coated stents. Recent *in vitro* data was shown, which demonstrated that the blood-submerged coated stents remained free of blood cell coagulation, and confirmed that the heparin was indeed active. The project would benefit from quantitative microscopic structure measurements to complement the more macroscopic studies and biological assays. The project would also benefit from grazing-incidence small-angle-X-ray scattering studies at the ESRF, to probe the microscopic in-plane structure of the biomolecular over layer. Neutron or synchrotron X-ray reflectivity measurements would further allow the density normal to the heparin-solid interface to be determined. This would be a very accurate measurement of the surface coverage parameter, which most likely should correlate to the degree of biocompatibility of the coated stent (a key measure of the success of the project).

The multi-disciplinary aspects of this ongoing project were evident, where aside from the physical measurements, the molecular cell biologists and medical scientists at the University are studying and optimising the immunological responses of the stents. The project has a very good scientific quality with highly competent principle investigators.

A very interesting multi-disciplinary project in the group of Reine Wallenberg *et al.* at Lund University is centred on the elucidation of the role of a class of lipids in insulin secretion of islets of Langerhans in response to glucose. Aberrations in the intracellular biological activity of these lipids (which under healthy conditions are associated with lipid metabolism in cells in the storage and eventual mobilisation of the enzyme modified signalling lipid) are implicated in Type II diabetes, which sets in at later stages in life. Thus, the project combines research from physical sciences and molecular cell biology and may potentially impact an important societal medical problem.

Excellent work is being conducted by a team of researchers (Kajsa Uvdal, Bo Liedberg, Ingemar Lundström *et al.*) at Linköping University in research on natural nanosystems for the development of biosensors, biomimetic materials synthesis, and nanomaterials development for biomedical applications. This group has a strong multi-disciplinary collaboration with Faculty from the departments of chemistry, biology, and medicine. The team has initiated two new initiatives to encourage multi-disciplinary work through the development of new graduate-level courses for the education

of students in more than one discipline, and the “twinning” of graduate students from two groups (e.g., physics and biology or medicine).

An example of an innovative project from the group includes the development of biosensors with the use of a biological cellular system, which contains cells with melanosomes, which are either dispersed in the cell body, or in response to a chemical input, travel to the cell centre. The distribution of the melanosomes within the cell determines whether they are transparent (melanosomes confined to the cell centre lead to negligible light scattering) or opaque (melanosomes dispersed in cell scatter light strongly). Thus, the on/off light scattering from a collection of cells is in response to the absence/presence of the chemical (and forms the basis of sensing the molecule). The project is carried out with medical scientists from the hospital, who provide the cell culturing facilities, as well as the genetic engineering expertise to grow mutant cells, which are able to detect the chemicals of interest, including pharmacological drugs. This is a very original project.

The biomimetic materials science effort by the team is centred on several novel projects. One was on understanding the molecular basis of sharkskin in order to produce a synthetic mimic exhibiting ultra-low friction coefficient properties. Other projects included the development of biologically inspired antifreeze interfaces with self-assembled glyco-peptides, the use of mesoporous materials for drug encapsulation and release, and the synthesis of helix-loop-helix peptides for sensing of proteins.

A very impressive project in this group is centred on developing magnetic nanoparticles ( $Gd_2O_3$ ) as a magnetic resonance imaging contrast agent. The long-term goal of this project is to develop cell-level imaging techniques, which would have potentially important applications in the early detection of brain tumours. This is an example of a successful research project between Faculty from the physical sciences and from medicine.

Overall, the ongoing projects by this team are original, have very high intellectual merit, and are potentially very important to health-related societal issues.

Olle Inganäs *et al.* at Linköping University are conducting research on the development and characterisation of organic photovoltaics and the self-assembly of complimentary macromolecular complexes for biomolecule detection. While the work of this group appears very good/excellent, nevertheless, in many instances the science is following what was first done outside of Sweden. For example, the detection of DNA oligomer sequences after complexation with a zwitterionic macromolecule via fluorescence detection was first developed in the Heeger and Bazan laboratories at the University of California at Santa Barbara. Nevertheless, a significant advantage of this group at Linköping is the strong collaboration with local synthetic

chemistry groups. This is enabling them to explore the possibilities of detecting a broad range of medically important biological molecules, for example, miss-folded insulin proteins and proteins implicated in neurodegenerative diseases. The principle investigator is clearly competent to carry out the proposed research.

### ***Biophysics***

The group of Bengt Kasemo *et al.* at Chalmers University of Technology has a long tradition of excellent research accomplishments in surface science (still ongoing) with new research programmes in biophysics. Some parts of the project may be better classified as biomedical engineering in collaboration with biology and medical scientists.

One of the main efforts in the group is on fundamental biophysical studies, aimed at elucidating the parameters, which determine how lipid vesicles spread on surfaces, and the distinct structures that are formed at the solid/lipid interface. For example, at least three distinct structures, which include supported bilayers, supported monolayers, or non-spreading surface adhered vesicles, are observed. Most recently, experiments from the group suggest that electrostatics plays a dominant role in stabilising the fully wetted supported lipid bilayer state. The group's studies are focused on understanding both the kinetics of bilayer formation after vesicle attachment (i.e., the mechanism of rupture or pore formation preceding wetting of the support by lipids), and the characterisation of the final equilibrium state (e.g., the final thickness of the bilayer resulting from considerations of equilibrium surface forces, the tilt angle of the lipids, and the chain ordering state of the bilayer).

The supported bilayer state is of primary interest in applications because it is required for the development of supported "functionalised" lipid bilayers. The functionalisation results from the presence of added peptide molecules anchored through a hydrophobic moiety within the environment of the lipid bilayer and protruding outward. Most recently, in collaboration with biologists and medical researchers they have demonstrated that they are able to produce functionalised supported bilayers with an oligo-peptide sequence specifically binding stem cells. The long-range goal of this project is to design functionalised supported bilayers for the attachment and differentiation of stem cells into different cell types for the purpose of medical therapeutics (e.g., to produce neurons to replace damaged nerve cells resulting from either neurodegenerative diseases or injury).

In summary, the investigators of this research group are highly innovative as is clearly shown in past work and the proposed work on surface control of stem cell differentiation. The intellectual merits of the ongoing and proposed research projects in this group are very high.

### ***Soft Matter***

Excellent/outstanding research is going on in the group of Lars Börjesson *et al.* at Chalmers University of Technology, in soft condensed matter physics. Their long-term goal is to set-up Chalmers (CTH) as the “centre for soft condensed matter” in Sweden. They propose to do this through an inclusive approach by including in their centre the research activities of their collaborators from all departments working on colloidal science and computational chemistry. The group has a solid track record of fundamental studies of the dynamics of glassy systems near the glass transition. They are careful in their choice of systems, for example, to simplify the physics of the problem; they are studying glass dynamics in relatively simple molecules (special alcohols) where H-bonding is not a dominant feature of the intermolecular interactions. More recently, they have been studying the glass transition under confined conditions, for example, water intercalated in clays, where they study the dynamics as a function of the number of water layers. In elegant experiments, they have shown the difference in dynamics, where rotational and translational degrees of freedom are drastically slowed down, as they go from two to a single layer of water. These latter studies may be viewed as model systems to aid our understanding of the behaviour of water molecules surrounding biologically active molecules.

The group has more recent research efforts on studies aimed at elucidating the fundamental dynamical behaviour in gels, colloids, and thin polymeric films by comparing to the dynamics of glassy systems (where the group has extensive experience). A novel and more applied project involves developing biosensors using nanoparticles with coated sensing biomolecules (i.e., playing the role of an antigen), which exhibit a shift in spectral response (thus forming the basis of a sensor) upon binding the protein of interest (i.e., the antibody).

The Salaneck group at Linköping University has a long history of excellent research on the electronic structure of conjugated polymers, doping of conjugated polymers and model molecules, and hybrid interfaces in polymer electronics. The most recent ongoing and proposed work is on studies of semiconductors for polymer-based electronics and displays. The group primarily focuses on the study of the physics and materials science of polymer surfaces and hybrid interfaces. No device work is done at Linköping and many materials are obtained through collaborations with international groups.

### ***New Techniques Development for Soft and Biological Matter***

Biomedical and X-ray Physics, the group of Hans Hertz *et al.* at the KTH is engaged in outstanding and truly innovative research on developing novel

X-rays, optics, and acoustics-based techniques with applications in biophysics and soft matter, biology, and medicine (i.e., perhaps not central within CMP area). The well-known work from this group is the development of “in-house” soft X-ray microscopes for direct imaging of cells and intracellular components. The development of the microscope has depended on many innovations by the principle investigator in developing liquid-jet-target laser-plasma soft X-ray sources and X-ray diffractive optics using transmission zone plates. The impact of this microscope in cell imaging with about a 30 nm resolution is expected to be very high, precisely because of the fact that such a microscope will be easily available for routine operation at University laboratories (in comparison to existing soft X-ray microscopes, which are based on synchrotron radiation facilities).

Most recently, the principle investigator and his group have developed a hard X-ray source emanating from liquid tin jets under electron beam bombardment. Because of the inherent small source size of about 30  $\mu\text{m}^2$  (limited by the electron-beam size), the X-ray brightness is between two to three orders of magnitude larger than commercially available rotating anode X-ray sources. Results from this ongoing work were presented during the review and the production of patterned surfaces containing distinct 25 nm lines (at the cutting edge of spatial resolution) demonstrates the impact this work will have worldwide in nanolithography, which is currently feasible only at very expensive national synchrotron light sources.

### *Quantitative Electron Microscopy Methods for Microscopic Structure Determination*

The work of Osamu Terasaki at Stockholm University on structural characterisation of mesoporous materials is clearly at the forefront of this research area worldwide. Over the years, the investigator has assembled an impressive set of collaborations with other internationally renowned materials chemists. A major area of current and proposed future research is the synthesis of nanocluster-arrays within the cavities of porous zeolites and mesoporous crystals. The materials are expected to exhibit important electronic and optical properties resulting from the quantum mechanical coupling of clusters arranged on periodic structures.

By far the most important contribution of Terasaki has been the development of electron microscopy methods for the quantitative microscopic structure determination of advanced materials, including mesoporous materials. The methods innovated by Terasaki for structure determination are applicable to both soft and hard materials and are examples of a tour-de-force of experimental ingenuity.

## Future Perspectives

Biomaterials research in Sweden appears very healthy, with many groups participating in internationally recognised research. However, the Panel did note that the majority of research in these groups, while very important, has a heavy emphasis on applications.

Many important examples of interactions between physical scientists and molecular cell biologist were presented during the review. For example, Wallenberg *et al.* at Lund University are working on biomedical problems related Type II diabetes, and we encourage the Research Council to continue funding of these types of projects. The ongoing and proposed projects in the biomaterials/materials chemistry effort at the KTH (Muhammed *et al.*) have a high scientific and societal value to medicine. The funding level by the Research Council appears to be adequate and appropriate. One way in which the Panel sees potential for even further improvement in this research project would be collaboration with the group of Osamu Terasaki at Stockholm University, for direct imaging with electron microscopy of the partially ordered materials prepared by Mamoun Muhammed.

Although traditional soft condensed matter research (i.e., involving non-biological materials such as colloids and foams) does not constitute a large research effort in Sweden, nevertheless, excellent research is being conducted by the group of Lars Börjesson *et al.* at Chalmers. Indeed, the research in this group has its main emphasis on basic science and the work is visible at the international level and fully deserving of steady Research Council-funding. Some soft matter efforts in Sweden are well connected to industry. Most prominently, Salaneck group's research effort on conducting polymers at Linköping University is recognised by industry worldwide, with Merck Chemicals and Dupont providing support. The group has also funding from the SSF and the EU. The quality of research in this group is clearly world class, but the Expert Panel notes the very important underpinning role that the Swedish Research Council-funding plays for this group.

The research area which was most conspicuous by its absence in the research covered by the Panel's review of Sweden's soft matter effort, is in the physics of liquid crystals. Both De Gennes' liquid crystal textbook and the more recent book by P. Chaikin and T. C. Lubensky clearly show that liquid crystal phases and phase transitions have presented us with a very large number of experimental systems (more than any other condensed matter system) to test and confirm, i.e., the major theoretical concepts in physics associated with "spontaneously broken symmetry" systems and the appearance of Goldstone modes over the last three decades (see, e.g., the introduction to major themes in condensed matter theory).

Furthermore, it was not clear whether the work reviewed by the Expert Panel within biophysics fully reflected the entire scope of the effort in this field in Sweden, but the Panel certainly noticed substantial scope for feasible expansion. With some notable exceptions (e.g., the work emerging from the group of Bengt Kasemo *et al.* at Chalmers University of Technology), very few groups in condensed matter physics are working on understanding the physics of membranes, protein self-assembly, and single biological molecules; these are areas, which are extremely active at the worldwide level.

The Panel was very impressed by new techniques development for soft matter and biological matter by several groups. The group of Hans Hertz *et al.* at the KTH is engaged in state-of-the-art development of “in-house” X-ray microscopes and hard X-ray sources. The investigator is a world-renowned researcher and among a handful of the most gifted X-ray physicists worldwide, including Janos Kirz (Professor at SUNY-Stony Brook and Acting Director of the Advanced Light Source at the Lawrence Berkeley Laboratories) and W. Yun (CEO of XRADIA Inc.; the company markets commercial rotating anode X-ray microscopes based on patents held by W. Yun). Osamu Terasaki at Stockholm University is among the leaders in developing methods for quantitative structure determination with electron microscopy. These are outstanding techniques development projects, which deserve strong ongoing support.

It appeared to the Expert Panel that some groups were understaffed considering the number of ongoing projects. For example, multiple very ambitious projects are going on and proposed by Olle Inganäs *et al.* at Linköping University (organic photovoltaics, biosensors development, detection of neurodegenerative misfolded proteins), although the effort comprises a single professor. Thus, while the projects are scientifically important, they may only be viable with a significant level of funding.

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*Swedish National Facilities*, Swedish Research Council (VR), 2002

*International Evaluation of Biotechnology*, Swedish Research Council (VR), 2003

# APPENDIX 1

## List of Evaluated Grant Holders and Groups

Surname	First name	Division/Department (or corresponding)	Univ	Internet address
Fogelström	Mikael	Applied Quantum Physics/Microtechnology an Nanoscience	CTH	<a href="http://www.mc2.chalmers.se/mcz/aqpl/">www.mc2.chalmers.se/mcz/aqpl/</a>
Shumeiko	Vitaly	Applied Quantum Physics/Microtechnology an Nanoscience	CTH	<a href="http://www.mc2.chalmers.se/mcz/aqpl/">www.mc2.chalmers.se/mcz/aqpl/</a>
Wendin	Göran	Applied Quantum Physics/Microtechnology an Nanoscience	CTH	<a href="http://www.mc2.chalmers.se/mcz/aqpl/">www.mc2.chalmers.se/mcz/aqpl/</a>
Campbell	Eleanor	Atomic Physics/Experimental Physics	GU	<a href="http://www.fy.chalmers.se/atom/">www.fy.chalmers.se/atom/</a>
Popok	Vladimir	Atomic Physics/Experimental Physics	GU	<a href="http://www.fy.chalmers.se/atom/">www.fy.chalmers.se/atom/</a>
Chakarov	Dinko	Chemical Physics/Applied Physics	CTH	<a href="http://www.fy.chalmers.se/kemfys">www.fy.chalmers.se/kemfys</a>
Fridell	Erik	Chemical Physics/Applied Physics	CTH	<a href="http://www.fy.chalmers.se/kemfys">www.fy.chalmers.se/kemfys</a>
Kasemo	Bengt	Chemical Physics/Applied Physics	CTH	<a href="http://www.fy.chalmers.se/kemfys">www.fy.chalmers.se/kemfys</a>
Bergman	Rikard	Condensed matter physics/Applied Physics	CTH	<a href="http://www.fy.chalmers.se/cmp/">www.fy.chalmers.se/cmp/</a>
Börjesson	Lars	Condensed matter physics/Applied Physics	CTH	<a href="http://www.fy.chalmers.se/cmp/">www.fy.chalmers.se/cmp/</a>
Jacobsson	Per	Condensed matter physics/Applied Physics	CTH	<a href="http://www.fy.chalmers.se/cmp/">www.fy.chalmers.se/cmp/</a>
Käll	Mikael	Condensed matter physics/Applied Physics	CTH	<a href="http://www.fy.chalmers.se/cmp/">www.fy.chalmers.se/cmp/</a>
Matic	Aleksandar	Condensed matter physics/Applied Physics	CTH	<a href="http://www.fy.chalmers.se/cmp/">www.fy.chalmers.se/cmp/</a>
Swenson	Jan	Condensed matter physics/Applied Physics	CTH	<a href="http://www.fy.chalmers.se/cmp/">www.fy.chalmers.se/cmp/</a>
Apell	Peter	Condensed matter theory/Applied Physics	CTH	<a href="http://www.fy.chalmers.se/cmt/">www.fy.chalmers.se/cmt/</a>
Gorelik	Leonid	Condensed matter theory/Applied Physics	CTH	<a href="http://www.fy.chalmers.se/cmt/">www.fy.chalmers.se/cmt/</a>
Jonson	Mats	Condensed matter theory/Applied Physics	CTH	<a href="http://www.fy.chalmers.se/cmt/">www.fy.chalmers.se/cmt/</a>
Kimaret	Jari	Condensed matter theory/Applied Physics	CTH	<a href="http://www.fy.chalmers.se/cmt/">www.fy.chalmers.se/cmt/</a>
Shekhter	Robert	Condensed matter theory/Applied Physics	CTH	<a href="http://www.fy.chalmers.se/cmt/">www.fy.chalmers.se/cmt/</a>
Kanski	Janusz	Electronic structure of condensed matter/Experimental Physics	CTH	<a href="http://www.fy.chalmers.se/cme">www.fy.chalmers.se/cme</a>
Nilsson	Per-Olof	Electronic structure of condensed matter/Experimental Physics	CTH	<a href="http://www.fy.chalmers.se/cme">www.fy.chalmers.se/cme</a>
Starnberg	Hans	Electronic structure of condensed matter/Experimental Physics	GU	<a href="http://www.fy.chalmers.se/cme">www.fy.chalmers.se/cme</a>
Gao	Shiwu	Materials and Surface theory/Applied Physics	CTH	<a href="http://fy.chalmers.se/ap/mst">http://fy.chalmers.se/ap/mst</a>
Lundqvist	Bengt	Materials and Surface theory/Applied Physics	CTH	<a href="http://fy.chalmers.se/ap/mst">http://fy.chalmers.se/ap/mst</a>

<b>Surname</b>	<b>First name</b>	<b>Division/Department (or corresponding)</b>	<b>Univ</b>	<b>Internet address</b>
Persson	Mats	Materials and Surface theory/Applied Physics	C:TH	<a href="http://fy.chalmers.se/ap/mst">http://fy.chalmers.se/ap/mst</a>
Schröder	Elsebeth	Materials and Surface theory/Applied Physics	C:TH	<a href="http://fy.chalmers.se/ap/mst">http://fy.chalmers.se/ap/mst</a>
Wahnström	Göran	Materials and Surface theory/Applied Physics	C:TH	<a href="http://fy.chalmers.se/ap/mst">http://fy.chalmers.se/ap/mst</a>
Olsson	Eva	Microscopy and Microanalysis/Experimental Physics	C:TH	<a href="http://fy.chalmers.se/microscopy/">http://fy.chalmers.se/microscopy/</a>
Andersson	Thorvald	Microwave electronics/Microtechnology an Nanoscience	C:TH	<a href="http://fy.chalmers.se/mbe/">http://fy.chalmers.se/mbe/</a>
Rosén	Arne	Molecular Physics Group/Experimental Physics	C:TH	<a href="http://fy.chalmers.se/f3c/">http://fy.chalmers.se/f3c/</a>
Bolton	Kim	Molecular Physics Group/Experimental Physics	GU	<a href="http://fy.chalmers.se/f3c/">http://fy.chalmers.se/f3c/</a>
Willander	Magnus	Physical Electronics and Photonics/Microtechnology an Nanoscience	C:TH	<a href="http://fy.chalmers.se/pep/">http://fy.chalmers.se/pep/</a>
Claeson	Tord	Quantum Device Physics/Microtechnology an Nanoscience	C:TH	<a href="http://www.mcz.chalmers.se/mcz/qdp/">www.mcz.chalmers.se/mcz/qdp/</a>
Delising	Per	Quantum Device Physics/Microtechnology an Nanoscience	C:TH	<a href="http://www.mcz.chalmers.se/mcz/qdp/">www.mcz.chalmers.se/mcz/qdp/</a>
Kidyarova-Shevchenko	Anna	Quantum Device Physics/Microtechnology an Nanoscience	C:TH	<a href="http://www.mcz.chalmers.se/mcz/qdp/">www.mcz.chalmers.se/mcz/qdp/</a>
Kuzmin	Leonid	Quantum Device Physics/Microtechnology an Nanoscience	C:TH	<a href="http://www.mcz.chalmers.se/mcz/qdp/">www.mcz.chalmers.se/mcz/qdp/</a>
Lombardi	Floriana	Quantum Device Physics/Microtechnology an Nanoscience	C:TH	<a href="http://www.mcz.chalmers.se/mcz/qdp/">www.mcz.chalmers.se/mcz/qdp/</a>
Yurgens	August	Quantum Device Physics/Microtechnology an Nanoscience	C:TH	<a href="http://www.mcz.chalmers.se/mcz/qdp/">www.mcz.chalmers.se/mcz/qdp/</a>
Hanson	Maj	Solid state physics/Experimental Physics	C:TH	<a href="http://www.fy.chalmers.se/solidstatephysics/">www.fy.chalmers.se/solidstatephysics/</a>
Hellsing	Bo	Solid state physics/Experimental Physics	C:TH	<a href="http://www.fy.chalmers.se/solidstatephysics/">www.fy.chalmers.se/solidstatephysics/</a>
Lindgren	Stig-Åke	Solid state physics/Experimental Physics	C:TH	<a href="http://www.fy.chalmers.se/solidstatephysics/">www.fy.chalmers.se/solidstatephysics/</a>
Svensson	Krister	Solid state physics/Experimental Physics	C:TH	<a href="http://www.fy.chalmers.se/solidstatephysics/">www.fy.chalmers.se/solidstatephysics/</a>
Walldén	Lars	Solid state physics/Experimental Physics	C:TH	<a href="http://www.fy.chalmers.se/solidstatephysics/">www.fy.chalmers.se/solidstatephysics/</a>
Eggert	Sebastian	Solid State Theory/Theoretical Physics	C:TH	<a href="http://fy.chalmers.se/tp/fasta">http://fy.chalmers.se/tp/fasta</a>
Granath	Mats	Solid State Theory/Theoretical Physics	C:TH	<a href="http://fy.chalmers.se/tp/fasta">http://fy.chalmers.se/tp/fasta</a>
Mehlig	Bernhard	Solid State Theory/Theoretical Physics	C:TH	<a href="http://fy.chalmers.se/tp/fasta">http://fy.chalmers.se/tp/fasta</a>
Sjögren	Lennart	Solid State Theory/Theoretical Physics	C:TH	<a href="http://fy.chalmers.se/tp/fasta">http://fy.chalmers.se/tp/fasta</a>

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Östlund	Stellan	Solid State Theory/Theoretical Physics	CTH	<a href="http://fy.chalmers.se/tp/fasta">http://fy.chalmers.se/tp/fasta</a>
Johannesson	Henrik	Solid State Theory/Theoretical Physics	GU	<a href="http://fy.chalmers.se/tp/fasta">http://fy.chalmers.se/tp/fasta</a>
Palmqvist	Anders	Applied Surface Chemistry/Chemical Engineering	CTH	<a href="http://www.surfchem.chalmers.se/">www.surfchem.chalmers.se/</a>
Andersson	Stig	Surface physics/Applied Physics	CTH	<a href="http://fy.chalmers.se/ap/sp/">http://fy.chalmers.se/ap/sp/</a>
Delin	Anna	Applied Materials Physics/Department of Materials Science	KTH	<a href="http://www.mse.kth.se">www.mse.kth.se</a>
Belonoshko	Anatoly	Applied Materials Physics/Department of Materials Science	KTH	<a href="http://www.mse.kth.se">www.mse.kth.se</a>
Persson	Clas	Applied Materials Physics/Department of Materials Science	KTH	<a href="http://www.mse.kth.se">www.mse.kth.se</a>
Hertz	Hans	Biomedical and X-ray Physics/Physics/	KTH	<a href="http://www.biox.kth.se">www.biox.kth.se</a>
Andersson	Magnus	Condensed Matter Physics/Laboratory of Solid State Devices/IMIT	KTH	<a href="http://www.ftf.kth.se/">www.ftf.kth.se/</a>
Grishin	Alexander	Condensed Matter Physics/Laboratory of Solid State Devices/IMIT	KTH	<a href="http://www.ftf.kth.se/">www.ftf.kth.se/</a>
Rapp	Östen	Condensed Matter Physics/Laboratory of Solid State Devices/IMIT	KTH	<a href="http://www.ftf.kth.se/">www.ftf.kth.se/</a>
Henelius	Patrik	Condensed matter theory/Physics	KTH	<a href="http://condmat.physics.kth.se">condmat.physics.kth.se</a>
Lidmar	Jack	Condensed matter theory/Physics	KTH	<a href="http://condmat.physics.kth.se">condmat.physics.kth.se</a>
Rosengren	Anders	Condensed matter theory/Physics	KTH	<a href="http://condmat.physics.kth.se">condmat.physics.kth.se</a>
Wallin	Mats	Condensed matter theory/Physics	KTH	<a href="http://condmat.physics.kth.se">condmat.physics.kth.se</a>
Hansson	Hans	Quantum and Field Theory/Department of Physics	SU	<a href="http://www.kof.physto.se/">www.kof.physto.se/</a>
Karlhede	Anders	Quantum and Field Theory/Department of Physics	SU	<a href="http://www.kof.physto.se/">www.kof.physto.se/</a>
Johnsson	Mats	Inorganic Chemistry/Department of Inorganic, Physical and Structural Chemistry	SU	<a href="http://www.fos.su.se">www.fos.su.se</a>
Lidin	Sven	Inorganic Chemistry/Department of Inorganic, Physical and Structural Chemistry	SU	<a href="http://www.fos.su.se">www.fos.su.se</a>
Terasaki	Osamu	Structural Chemistry/Department of Inorganic, Physical and Structural Chemistry	SU	<a href="http://www.fos.su.se">www.fos.su.se</a>

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Ekenberg	Ulf	Laboratory of Photonics and Microwave Engineering/OPQ/IMIT/	KTH	www.imit.kth.se/
Muhammed Mamoun		Materials Chemistry/Institutionen för materialvetenskap	KTH	http://web.mse.kth.se/matchem/
Göthelid	Mats	Material Physics/Laboratory of Materials and Semiconductor Physics/IMIT/	KTH	www.imit.kth.se/
Karlsson	Ulf	Material Physics/Laboratory of Materials and Semiconductor Physics/IMIT/	KTH	www.imit.kth.se/
Linnarsson	Margareta	Solid State Electronics/Laboratory of Materials and Semiconductor Physics/IMIT	KTH	www.imit.kth.se/
Nordell	Nils	Semiconductor Laboratory/IMIT	KTH	www.imit.kth.se/
Tjernberg	Oscar	Material Physics/Laboratory of Materials and Semiconductor Physics/IMIT/	KTH	www.imit.kth.se/
Zhang	Shi-Li	Device Technology/Laboratory of Solid State Devices/IMIT	KTH	www.imit.kth.se/
Åkermark	Torbjörn	Material Physics/Laboratory of Materials and Semiconductor Physics/IMIT/	KTH	www.imit.kth.se/
Dzugutov	Mikhail	NADA/KTH	KTH	www.nada.kth.se/~mik/
Haviland	David	Nanostructure physics/Fysik	KTH	www.nanophys.kth.se
Korenivski	Vladislav	Nanostructure physics/Fysik	KTH	www.nanophys.kth.se
Nilsson	Anders	Quantum chemistry/Fysikum	SU	www-ssrl.slac.stanford.edu/ nilssonsgroup/
Arwin	Hans	Applied optics/Applied physics/IFM	LiU	www.ifm.liu.se/applopt/
Uvdal	Kajsa	Sensor science and molecular physics/Applied Physics/IFM	LiU	www.ifm.liu.se/applphys/sensor/
Liedberg	Bo	S-SCENCE/Applied Physics/IFM	LiU	www.ifm.liu.se/applphys/sensor/
Lundström	Ingemar	S-SCENCE/Applied Physics/IFM	LiU	www.ifm.liu.se/~ingemar/

Surname	First name	Division/Department (or corresponding)	Univ	Internet address
Inganäs	Olle	Biomolecular and organic electronics/Applied Physics/IFM	LiU	www.ifm.liu.se/biorgel
Buyanova	Irina	Material Science Division/Material Physics/IFM	LiU	www.ifm.liu.se/Matephys/
Chen	Weimin	Material Science Division/Material Physics/IFM	LiU	www.ifm.liu.se/Matephys/
Holtz	Per-Olof	Material Science Division/Material Physics/IFM	LiU	www.ifm.liu.se/Matephys/
Johansson	Leif	Material Science Division/Material Physics/IFM	LiU	www.ifm.liu.se/Matephys/
Monemar	Bo	Material Science Division/Material Physics/IFM	LiU	www.ifm.liu.se/Matephys/
Weman	Helge	Material Science Division/Material Physics/IFM	LiU	www.ifm.liu.se/Matephys/
Zozoulenko	Igor	Mesoscopic Physics and Nanoelectronics/Campus Norrköping	LiU	www.itn.liu.se/~igozo/mes_nano.htm
Fahlman	Mats	Organic physics/Inst. För teknik och naturvetenskap/Norrköping	LiU	www.itn.liu.se/~matfa/OrgPhys.htm
Erlandsson	Ragnar	Scanning Probe Microscopy/Applied physics/IFM	LiU	www.ifm.liu.se/AppPhys/spm/
Hansson	Göran	Surface and semiconductor physics/Material Physics/IFM	LiU	www.ifm.liu.se/semiphys/
Ni	Wei-Xin	Surface and semiconductor physics/Material Physics/IFM	LiU	www.ifm.liu.se/semiphys/
Uhrberg	Roger	Surface and semiconductor physics/Material Physics/IFM	LiU	www.ifm.liu.se/semiphys/
Friedlein	Rainer	Surface physics and chemistry/Material Physics/IFM	LiU	www.ifm.liu.se/surfphys/
Salaneck	William	Surface physics and chemistry/Material Physics/IFM	LiU	www.ifm.liu.se/surfphys/
Abrikosov	Igor	Theory and modeling/IFM	LiU	www.ifm.liu.se/theomod/
Berggren	Karl-Fredrik	Theory and modeling/IFM	LiU	www.ifm.liu.se/theomod/
Boström	Mathias	Theory and modeling/IFM	LiU	www.ifm.liu.se/theomod/
Johansson	Magnus	Theory and modeling/IFM	LiU	www.ifm.liu.se/theomod/
Munger	Peter	Theory and modeling/IFM	LiU	www.ifm.liu.se/theomod/
Riklund	Rolf	Theory and modeling/IFM	LiU	www.ifm.liu.se/theomod/
Sernelius	Bo E.	Theory and modeling/IFM	LiU	www.ifm.liu.se/theomod/
Simak	Sergey	Theory and modeling/IFM	LiU	www.ifm.liu.se/theomod/
Stafström	Sven	Theory and modeling/IFM	LiU	www.ifm.liu.se/theomod/

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Helmerson	Ulf	Thin film physics/Material physics/IFM	LiU	www.ifm.liu.se/thinfilm/
Hultman	Lars	Thin film physics/Material physics/IFM	LiU	www.ifm.liu.se/thinfilm/
Kröll	Stefan	Atomic Physics/Fysicum/LTH	LTH	www-atom.fysik.lth.se/PhotonEcho/
Uvdal	Per	Chemical physics/Chemical Center	LU	http://spider.chemphys.lu.se/
Wallenberg	Reine	Materials chemistry/Chemical Center	LU	www.materialekemi.lth.se
Guhr	Thomas	Mathematical Physics/Fysicum/LTH	LTH	www.matfys.lth.se
Reimann	Stephanie	Mathematical Physics/Fysicum/LTH	LTH	www.matfys.lth.se
Deppert	Knut	Solid state theory/Fysicum/LTH	LTH	www.ffl.lth.se
Gustafsson	Anders	Solid state theory/Fysicum/LTH	LTH	www.ffl.lth.se
Hessman	Dan	Solid state theory/Fysicum/LTH	LU	www.ftf.lth.se
Montelius	Lars	Solid state theory/Fysicum/LTH	LU	www.ftf.lth.se
Pistol	Mats-Erik	Solid state theory/Fysicum/LTH	LU	www.ftf.lth.se
Samuelson	Lars	Solid state theory/Fysicum/LTH	LU	www.ftf.lth.se
Xu	Hongqi	Solid state theory/Fysicum/LTH	LU	www.ftf.lth.se
Almbladh	Carl-Olof	Solid state theory/Fysicum/LU	LU	www.teorfys.lu.se
Chao	Koung-An	Solid state theory/Fysicum/LU	LU	www.teorfys.lu.se
Andersen	Jesper	Synchrotron radiation research/Fysicum/LU	LU	www.sjrus.lu.se
Lindau	Ingolf	Synchrotron radiation research/Fysicum/LU	LU	www.sjrus.lu.se
Lundgren	Edvin	Synchrotron radiation research/Fysicum/LU	LU	www.sjrus.lu.se
Nyholm	Ralf	Maxlab	LU	www.maxlab.lu.se

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Andersson	Ove	Experimental physics/Department of Physics	UMU	www.phys.umu.se/nano_phys/
Ferry	Anders	Experimental physics/Department of Physics	UMU	www.phys.umu.se/nano_phys/
Makarova	Tatiana	Experimental physics/Department of Physics	UMU	www.phys.umu.se/nano_phys/
Sundqvist	Bertil	Experimental physics/Department of Physics	UMU	www.phys.umu.se/nano_phys/
Canali	Carlo Maria	Dep of Chemistry and Biomedical Sciences	HIK	www.hik.se/forskning/
Karlsson	Krister	HS Skövde	HIS	www.his.se
Johansson	Lars	Physics/University of Karlstad	KAU	www.ingvet.kau.se/fys/
Weber	Hans	Division of Physics/Department of mechanical engineering/Luleå	LTU	www.ltu.se
Olin	Håkan	Department of Engineering, Physics and Mathematics/MH	MH	www.tfm.mh.se/hakoli
Johansson	Peter	Solid State Theory/Physics/Örebro universitet	ORU	www.oru.se/nat/fysik
Olsson	Peter	Theoretical physics/Department of Physics	UMU	www.phys.umu.se/indexeng.htm
Rammer	Jørgen	Theoretical physics/Department of Physics	UMU	www.phys.umu.se/indexeng.htm
Mimnhagen	Petter	NORDITA/UMU	NORDITA	www.nordita.dk
Snuppen	Kim	NORDITA	NORDITA	www.nordita.dk
Ahuja	Rajeev	Condensed matter theory/Department of physics	UU	www.fysik4.fysik.uu.se
Johansson	Börije	Condensed matter theory/Department of physics	UU	www.fysik4.fysik.uu.se
Mirbt	Susanne	Condensed matter theory/Department of physics	UU	www.fysik4.fysik.uu.se
Lieberman	Michael	Condensed matter theory/Department of physics	UU	http://liii.fysik.uu.se
Rensmo	Håkan	Electron spectroscopy and molecular surface physics/ Department of physics	UU	www.fysik.uu.se/LiquidInterface/
Sandell	Anders	Electron spectroscopy and molecular surface physics/ Department of physics	UU	www.fysik.uu.se/LiquidInterface/
Siegbahn	Hans	Electron spectroscopy and molecular surface physics/ Department of physics	UU	www.fysik.uu.se/LiquidInterface/

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Fogelberg	Birger	Nuclear physics/Department of radiation sciences	UU	<a href="http://www.isv.uu.se/isv.html">www.isv.uu.se/isv.html</a>
Ebbsjö	Ingvar	Studsvik Neutron Research Laboratory/UU	UU	<a href="http://www.studsvik.uu.se">www.studsvik.uu.se</a>
Butorin	Sergei	Soft X-ray Physics/Department of physics	UU	<a href="http://usx218.fysik.uu.se/">http://usx218.fysik.uu.se/</a>
Duda	Laurent	Soft X-ray Physics/Department of physics	UU	<a href="http://usx218.fysik.uu.se/">http://usx218.fysik.uu.se/</a>
Magnusson	Martin	Soft X-ray Physics/Department of physics	UU	<a href="http://usx218.fysik.uu.se/">http://usx218.fysik.uu.se/</a>
Nordgren	Joseph	Soft X-ray Physics/Department of physics	UU	<a href="http://usx218.fysik.uu.se/">http://usx218.fysik.uu.se/</a>
Rubensson	Jan-Erik	Soft X-ray Physics/Department of physics	UU	<a href="http://usx218.fysik.uu.se/">http://usx218.fysik.uu.se/</a>
Nordblad	Per	Magnetism/Solid state physics/Department of Engineering Sciences	UU	<a href="http://www.angstrom.uu.se/magnetism/">www.angstrom.uu.se/magnetism/</a>
Svedlindh	Peter	Magnetism/Solid state physics/Department of Engineering Sciences	UU	<a href="http://www.angstrom.uu.se/magnetism/">www.angstrom.uu.se/magnetism/</a>
Heszler	Peter	Material optics/Solid state physics/Department of Engineering Sciences	UU	<a href="http://www.angstrom.uu.se/solidstatephysics/">www.angstrom.uu.se/solidstatephysics/</a>
Niklasson	Gunnar	Material optics/Solid state physics/Department of Engineering Sciences	UU	<a href="http://www.angstrom.uu.se/solidstatephysics/">www.angstrom.uu.se/solidstatephysics/</a>
Ribbing	Carl-Gustaf	Material optics/Solid state physics/Department of Engineering Sciences	UU	<a href="http://www.angstrom.uu.se/solidstatephysics/">www.angstrom.uu.se/solidstatephysics/</a>
Arvanitis	Dimitri	Surface physics/Department of physics	UU	<a href="http://fysik5.fysik.uu.se/">http://fysik5.fysik.uu.se/</a>
Hunter Dunn	Jonathan	Maxlab	LU	<a href="http://www.maxlab.lu.se/">www.maxlab.lu.se/</a>
Karis	Olof	Surface physics/Department of physics	UU	<a href="http://fysik5.fysik.uu.se/">http://fysik5.fysik.uu.se/</a>
Mårtensson	Nils	Surface physics/Department of physics	UU	<a href="http://fysik5.fysik.uu.se/">http://fysik5.fysik.uu.se/</a>
Puglia	Carla	Surface physics/Department of physics	UU	<a href="http://fysik5.fysik.uu.se/">http://fysik5.fysik.uu.se/</a>
Eriksson	Olle	Teoretisk magnetism/Department of physics	UU	<a href="http://www.fysik.uu.se/theomag">www.fysik.uu.se/theomag</a>
Nordström	Lars	Teoretisk magnetism/Department of physics	UU	<a href="http://www.fysik.uu.se/theomag">www.fysik.uu.se/theomag</a>

# APPENDIX 2

## Short Summaries of Group Activities

(In the same order as in the “list of groups” in the appendix above)

### CHALMERS UNIVERSITY OF TECHNOLOGY AND GÖTEBORG UNIVERSITY

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University: CTH  
Division: Applied Quantum Physics  
Head or representative: Vitaly Shumeiko  
Group composition (2004): Faculty 3 (Vitaly Shumeiko, Göran Wendin, and Mikael Fogelström);  
Post-docs 3; Ph.D. students 7

#### Summary of activities

Shumeiko and Wendin work together. One of their projects involves a readout mechanism for a “Cooper-pair box” type qubit, which involves coupling this qubit to a single-electron-transistor (i.e. another quantum dot in the Coulomb blockade regime containing an odd number of electrons). They have also proposed another type of superconducting qubit involving an Andreev bound state localised near a quantum point contact. They have worked on the theory of current transport in mesoscopic superconducting junctions based on a model of multiple Andreev reflection. Another recent activity involves electron transport through individual molecules. Fogelström, a recent addition to the group, appears to work independently from Shumeiko and Wendin on related topics including superconducting contacts and d-wave and p-wave superconductors. Most of the theoretical work of this group appears to be analytic (perturbation theory, proposal or devices and models, etc.) rather than involving large-scale numerical simulations.

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University: GU  
Division: Atomic Physics  
Head or representative: Eleanor Campbell  
Group composition (2004): Faculty 2 (Eleanor Campbell and Vladimir Popok);  
Post-docs 0; Ph.D. students 5

### Summary of Activities

The activities of this group focus on four topics: endohedral fullerenes, cluster ion implantation, metal/dielectric nanocomposites and carbon nanotubes. Due to the high stability and symmetry of  $C_{60}$ , endohedral  $C_{60}$  molecules ( $C_{60}$  containing a metal ion) are interesting from both a fundamental and applications oriented point of view. Ion cluster beams are a versatile tool for modification and processing of surfaces and near-surface layers on an atomistic scale. Implantation of clusters into various substrates has been carried out. Low-energy implantation has been used for synthesis of metal nanoparticles in dielectric matrices. The carbon nanotubes research is concentrated on the study of growth mechanisms using chemical vapour deposition and plasma-enhanced chemical vapour deposition techniques. Recent work is focusing on devices such as nanotubes-based relays for field effect transistors on silicon chips. The most significant contributions are: development of a technique to produce macroscopic quantities of endohedral fullerenes; characterisation of the properties of  $LiC_{60}$ ; study of non-linear optical properties of carbon nanotubes; production and characterisation of three-terminal carbon nanotube-based relay structures; use of high-power ion beams as an efficient practical means of polymer modification; evaluation of the laser ablation process.

University: CTH/GU  
 Division: Chemical Physics Group  
 Head or representative: Bengt Kasemo  
 Group composition (2004): Faculty 11: (Bengt Kasemo, Dinko Chakarov, Erik Fridell, Igor Zoric, Fredrik Höök, Duncan Sutherland, Ann Grant, Peter Thormählen, Henrik Grönbeck, Vladimir Zhdanov, and Ann-Sofie Andersson);  
 Post-docs 6; Ph.D. students 21

### Summary of Activities

This large group has its roots in mainstream surface science, but now covers three main themes: (i) basic surface physics, (ii) heterogeneous catalysis/nanocatalysis, and (iii) interfaces between biological and non-biological systems (Biological Physics and Biomaterials). Nanoscience and nanotechnology are now central in all of these activities. The more applied aspects of this work attract significant other funds through VINNOVA, the SSF and the European Commission. The more fundamental aspects of surface dynamics involve theoretical collaborations including the group of

Bengt Lundqvist at CTH. Much of the catalysis effort operates within the Competence Center for Catalysis (KCK), with a programme performing theoretical calculations and simulations of supported catalysts and their kinetics, and using IR spectroscopy to study catalytic reactions resolved in time and space. A so called Excellent Research Center (Excellentia forskningsmiljöer) is devoted to “preparation, characterisation, and property/process studies of combined hard and soft nano(bio)structures”.

University: CTH  
 Division: Condensed Matter Physics  
 Head or representative: Lars Börjesson  
 Group composition (2004): Faculty 11 (Lars Börjesson, Per Jacobsson, Mikael Käll, Aleksandar Matic, Rikard Bergman, Jan Swenson, Dennis Engberg, Denis Ostrovskii, Patrik Johansson, Hanna Matic, and Christer Svanberg);  
 Post-docs 5; Ph.D. students 15

### Summary of Activities

The group activities cover physics areas from soft and disordered condensed matter to strongly correlated oxides and biomolecules. A wide range of experimental facilities has been set-up to suit these areas.

The research activities can be divided into four main parts:

- physics of soft condensed matter and disordered materials, e.g., glass transition dynamics, glass structure, polymer dynamics, gel dynamics, anomalous low energy density of states, collective dynamics, dynamics in nanoconfined geometries, physics of biological matter, protein folding and dynamics, etc;
- physics of strongly correlated materials, e.g., high- $T_c$  superconductivity, colossal magnetoresistance, one-dimensional spin/charge dynamics of spin-ladder compounds, etc;
- physics of energy related materials, e.g., ion conducting glasses, polymer electrolytes, and proton conducting materials for potential use in future batteries and fuel cells;
- physics and biological applications of nano-optics (localised plasmon sensing, surface enhanced spectroscopy), development of advanced optical microscopy techniques for the life sciences.

**University:** CTH  
**Division:** Condensed Matter Theory  
**Head or representative:** Mats Jonson  
**Group composition (2004):** Faculty 8 (Mats Jonson, Peter Apell, Leonid Gorelik, Jari Kinaret, Zoran Konkoli, Robert Shekhter, Marina Voinova, and Tomas Carlsson);  
 Post-docs 0; Ph.D. students 5

### Summary of Activities

Several senior members of the group work closely together: Jonson, Shekhter, and Gorelik largely on projects in the nanoelectronics field. In particular, they proposed in 1998 a shuttle mechanism for charge transfer in Coulomb blockaded nanostructures. They proposed a somewhat related system in conjunction with other theorists in the U.S.A. and Russia in which the magnetic exchange interaction between ferromagnetic islands is modulated in a time-dependent fashion via gate voltages separating the two islands from a smaller ferromagnetic island in between them.

Kinaret works largely independently on somewhat similar problems using somewhat similar methods, although he tends to use additional technical methods, such as "Luttinger liquid" theory. Apell appears to work quite independently of the other senior group members on rather different subjects, especially involving light scattering or emission. In particular, he continues a long-standing collaboration with P. Johansson, a former student in this group, now at Örebro University. Apell is now vice-rector of Kristianstad University.

**University:** CTH  
**Division:** Electronic Structure of Condensed Matter  
**Head or representative:** Per-Olof Nilsson  
**Group composition (2004):** Faculty 3: (Per Olof Nilsson, Janusz Kanski, and Hans Starnberg);  
 Post-docs 0; Ph.D. students 3

### Summary of Activities

This group pursues experimental investigations of the electronic structure of mainly semiconductor materials and interfaces. One core activity is the application of core and valence level photoemission to such systems using MAX-lab beamlines, including studies to probe buried interfaces. Closely

related to this programme is the capability to investigate *in situ* MBE-grown semiconductor materials through a facility built up by the group, but permanently stationed at MAX-lab. In addition, to work on conventional III-V solids and interfaces, recent work has produced high-quality (GaMn)As magnetic semiconductors. A further theme is the study of reduced dimensionality in solid systems, and particularly layered transition metal dichalcogenides and intercalation in these systems. In addition to the use of photoemission to explore the electronic structure of these materials, recent work has included photoelectron microscopy to investigate the mechanisms of intercalation.

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University: CTH/ GU  
Division: Materials and Surface Theory  
Head or representative: Bengt Lundqvist  
Group composition (2004): Faculty 7 (Shiwu Gao, Per Hylgaard, Bengt Lundqvist, Mats Persson, Elsebeth Schröder, Sergei Simak, and Göran Wahnström);  
Post-docs 5; Ph.D. students 11

### Summary of Activities

The group engages in a range of activities related to the development of a framework for theoretical understanding of microscopic phenomena at solid surfaces, interfaces, and on nanostructures. For most part, they apply *ab initio* electronic structure calculations based on the density functional theory and supplemented by model Hamiltonians, as necessary. Lundqvist is one of the pioneers of techniques based on density functional theory, and continues to work on new developments to make the technique more robust and versatile. The group engages in accurate calculations of complex surfaces, with the aim of developing novel materials by design. Their calculations extend in general to complex surfaces and interfaces, such as metallic overlayers on oxide surfaces. Recent work also aims at explaining phenomena like the diffusion and reaction of light gases and water molecules on metal surfaces. Group members are also engaged in providing theoretical understanding of phenomena, such as atomic manipulation and thin film growth processes. An important strength of the group is the ability to work with some of the leading experimentalists in the field, code development and its application to novel complex phenomena is also a focus of the group's activities. While most of the work in the Lundqvist

group aims at addressing some of the leading fundamental issues in surface and materials science, they also find relevance in industrial application, for example the theoretical work on accurate determination of the structure of alumina that was featured on the cover page of the Journal of the American Ceramic Society.

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University: CTH/GU  
Division: Microscopy and Microanalysis  
Head or representative: Eva Olsson  
Group composition (2004): Faculty 1 (Eva Olsson);  
Post-docs 1; Ph.D. students 4

### Summary of Activities

The activities reported from this group only include activities and people having Research Council-supported grants. The overall research activity covers a much larger number of people and research projects. The Research Council-supported research activities of this group are directed towards electron microscopy-based studies of electrically active interfaces and photoactive and electrically active nanostructures. Electron holography, which provides information on the crystal field potential in a material, has been used for studying ZnO interfaces, including Schottky barrier formation and its correlation with the interface microstructure. Other materials of interest are magnetites and superconductors. The group is in this respect utilising their available instrumentation and expertise for addressing scientific questions of strong relevance for understanding the influence of the properties and grain structure or interface structure influence of these materials on the electrical behaviour. The group has been strongly involved in the TEM-STM holder, developed at Chalmers University, from the TEM side. In the near future, new electron microscopy instrumentation, which allows for 3D tomography, funded by the Knut & Alice Wallenberg Foundation, will be installed. The equipment is planned for studies of catalytic particles, nanostructures, interfaces, and clusters. The research plans also include materials studies at elevated temperatures, studies in wet environment, and TEM-STM studies of interfaces, defects, and nanostructured materials. For understanding the electronic properties of their experimental systems, the group is collaborating with theoretical groups at CTH performing DFT calculations.

**University:** CTH  
**Division:** Microwave Electronics  
**Head or representative:** Thorvald Andersson  
**Group composition (2004):** Faculty 1 (Thorvald Andersson);  
Post-docs 0; Ph.D. students 5

### Summary of Activities

The research is concentrated on basic issues of materials, processes, and technology, with focus on materials research, MBE-growth of device structures, and device processing. One objective of the group is to grow tailor-made AlGaIn/GaN heterostructures for high-speed and high-power HFET's and modulator devices. The material is analysed by XRD, SEM, AFM, Hall, CV, and theoretical models. They recently started work on evaporation growth, epitaxial growth, and spectroscopic studies of organic materials. Another part of the work is growth of organic molecules for OLED. The group investigates multi-layer structures and the interaction of a single layer with the substrate.

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**University:** CTH/GU  
**Division:** Molecular Physics  
**Head or representative:** Arne Rosén  
**Group composition (2004):** Faculty 3 (Arne Rosén, Mats Andersson,  
and Kim Bolton);  
Post-docs 1; Ph.D. students: 5

### Summary of Activities

The research in Arne Rosen's group of molecular physics at CTH, has been focused on a close co-operation between experimental and theoretical activities. One of the research areas of interest is studies of nanoscaled systems, such as atoms, atomic clusters, fullerenes, and carbon nanotubes, which is an interdisciplinary field bridging different areas of physics, chemistry and materials. Another research area is the use of different laser spectroscopic techniques for studies of catalytic reactions, in particular Planar Laser Induced Fluorescence, PLIF. The knowledge obtained from their two-dimensional imaging techniques has been the basis for their participation in a competence centre, Combustion Engine Research Centre, CERC, for studies of sprays in combustion, as well as the use of Photo Dynamic Diagnostics, PDD, and Photo Dynamic Therapy, PDT, for diagnosis and treatment of skin cancer.

**University:** CTH/GU  
**Division:** Physical Electronics and Photonics  
**Head or representative:** Magnus Willander  
**Group composition (2004):** Faculty 9 (M. Willander, Q.X. Zhao, O. Nur, E. Mamontov, Q.H. Hu, N. Calander, M. Karlsteen, M. Friesel, and Y. Fu); Post-docs 0; Ph.D. students 2

### Summary of Activities

The research activities of this group are versatile and related to a great number of subjects: mixed liquids, soft matter, and solid-state matter, such as the manipulation of a single molecule in water by electrical and optical forces (this structure also acted as a transistor built up by water); polarisation, relaxation and transport phenomena, such as the theoretical study of exciton (indirect) superfluidity, Bose-condensation and Wigner crystallisation, weak localisation, and the Shubnikov-de Haas oscillations. In materials research, the group is also active in various subjects concerning semiconductor systems: MBE growth of GaN and InAs dots on GaAs substrates; study of p-type doped GaAs as well as GaAs/AlGaAs and GaInNAs/GaAs quantum well structures; study of ZnO, in order to make device quality ZnO materials, mainly nanorods, for optical applications, lamps, and lasers.

**University:** CTH  
**Division:** Quantum Device Physics  
**Head or representative:** Per Delsing  
**Group composition (2004):** Faculty 10 (Per Delsing, Tord Claeson, Dag Winkler, Sergey Kubatkin, Leonid Kuzmin, Vladimir Krasnov, August Yurgens, Anna Kidiyarova-Shevchenko, Floriana Lombardi, and Tim Duty); Post-docs 9; Ph.D. students 26

### Summary of Activities

The scientific activities in this laboratory are conducted in three subgroups, parts of Quantum Device Physics:

- Quantum Devices and Oxide Electronics – QuOx (T.Claeson – D.Winkler, 20 – 25 persons). The main activities include complex oxide materials, Josephson junctions, ferroelectric heterostructures, spin devices based

on perovskite manganite ferromagnets, YBCO bi-epitaxial junctions, and pseudogap studies in HTSC.

- Experimental Mesoscopic Physics – EMP ( P.Delsing, 15 persons) Present activities are centred on single-electron transistors (SET), superconducting qubits, Coulomb blockade thermometry, metallic Andreev devices, and molecular electronics.
- The Bolometer group (L.Kuzmin, 5 persons). Development of supersensitive bolometers for radioastronomy research, superconductor-insulator-normal metal (SIN) tunnel junctions.

The High Frequency Digital group- HDFE (A.Kidiyarova-Shevchenko, 5 persons) is part of the Solid State Electronics Laboratory. The two main activities of this subgroup are the development of superconducting digital signal processors, and system on-chip solution for quantum computers based on the rapid single flux quantum logic.

University: CTH/GU  
 Division: Solid State Physics  
 Head or representative: Lars Walldén  
 Group composition (2004): Faculty 6 (Lars Walldén, Maj Hanson, Bo Hellsing, Olga Kazakova, Stig-Åke Lindgren, and Krister Svensson);  
 Post-docs 2; Ph.D. students 5

### Summary of Activities

This group covers a number of somewhat distinct topics. One such activity derives from the use of angle-resolved photoemission to characterise the electronic structure of solids and surfaces. The focus of recent work has been on very detailed investigations of quantum well states, notably for alkali metal films on graphite. Recent work in this area has made significant use of MAX-lab. A quite different topic is studies of the transport of electrons and solid matter in carbon nanotubes, exploiting a novel combination of STM and TEM, and including demonstrations of “nanopipette” functionality through electrodiffusion of Fe down carbon nanotubes. A third area is the study and development of nanostructured magnetic materials with novel properties, one ultimate aim is to find a prototype of an ultra-high density memory. In addition, theoretical studies are being pursued to study electron – phonon coupling and lifetime effects in a range of bulk and surface condensed matter phenomena.

**University:** CTH/GU  
**Division:** Solid State Theory  
**Head or representative:** Stellan Östlund  
**Group composition (2004):** Faculty 6 (Stellan Östlund, Henrik Johannesson, Lennart Sjögren, Sebastian Eggert, Bernhard Mehlig, and Mats Granath); Post-docs 0; Ph.D. students 3

### Summary of Activities

The group consists of six senior researchers, who work in different subfields in condensed matter physics; also under the loose heading “strongly correlated systems”. Östlund works in correlated quantum mechanical systems using density matrix re-normalisation group, symmetry analysis, and mean field methods. Mehlig concentrates on understanding the dynamics of inertial particles in random flows, patterns of genetic variations in human and mouse genome, and on optical and mechanical properties of nanostructured systems. Johannesson focuses on several aspects of strongly correlated systems, with particular emphasis on correlation effects from impurities, finite size and boundary effects, and field-theoretic description of fluctuation effects. Sjögren examines fluctuations of a physical variable that is not a Gaussian, as in the critical point of a second order phase transition. Granath’s work is also in correlated electron systems as in Mott-Hubbard insulator and stripe formation in high- $T_c$  superconductors. Eggert contributed (has now left Sweden) to the calculation of the Neel temperature in doped spin-1/2 compounds, predicts STM images in quantum wires, and considers effects of deformation and curvature in nanotubes.

**University:** CTH  
**Division:** Surface Chemistry  
**Head or representative:** Anders Palmqvist  
**Group composition (2004):** Faculty 1 (Anders Palmqvist); Post-docs 1; Ph.D. students 3

### Summary of Activities

While this group has a significant activity on lean de-NO<sub>x</sub> catalysis using mainly shape-selective zeolite catalysts, highly relevant to surface chemistry, this component of the work did not form part of the present review. The work covered by related Research Council-funding is concerned

with the synthesis and characterisation of nanostructured materials, using either self-assembly of molecules and particles or solvo-thermal routes, notably microporous semiconductors. The group routinely uses analytical techniques, such as SEM, TEM, N<sub>2</sub>-adsorption, XRD, SAXS, DLS, FTIR, UV-VIS, XPS, and NMR to follow the synthesis and to characterise their materials.

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University: CTH  
Division: Surface Physics  
Head or representative: Stig Andersson  
Group composition (2004): Faculty 2 (Stig Andersson and Curt Nyberg);  
Post-docs 0; Ph.D. students 2

#### Summary of Activities

This small group has its activities focused on the use of using atomic and molecular beam scattering methods and high-performance electron-loss spectroscopy, in order to elucidate fundamental microscopic aspects of elementary gas-surface processes. The work includes quantum scattering experiments; not only of H<sub>2</sub> and of D<sub>2</sub> from Cu and Al surfaces, but also of heavier species, and detailed studies of the vibrational and rotational states of molecular hydrogen on Cu at very low temperatures.

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University: KTH  
Division: Applied Materials Physics  
Head or representative: Börje Johansson  
Group composition (2004): Faculty 7 (Börje Johansson, Anna Delin, Anatoly Belonoshko, Clas Persson, Pavel Korzhavyi, Andrei Ruban, and Levente Vitos);  
Post-docs 1; Ph.D. students: 3

#### Summary of Activities

Börje Johansson has also started a research group at KTH with a more applied orientation to the application of electronic structure calculations to complex solids. One such application is to stainless steel. Carbides and

oxides of various types, doped oxides, and advanced metallic alloys with and without defects are other choices. An *ab initio* method based on exact muffin tin orbitals is combined with the coherent potential approximation to provide a feasible code for studying pressure-dependent properties of bulk and surface systems. Interaction potentials are also developed for application to more complex systems. Anna Delin's effort is in applying first principles techniques to understand magnetic properties of lower dimensional systems, particularly nanowires of 4d and 5d transition metals. The work of Belonoshko using classical molecular dynamics of melting and structural phase transition of several metals led to the scenario of shock wave propagation in extreme conditions. The two-phase simulation model introduced by Anatoly Belonoshko has become a standard in simulations of melting/freezing.

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University: KTH  
Division: Biomedical X-ray Physics  
Head or representative: Hans Hertz  
Group composition (2004): Faculty 4 (Hans Hertz, Kjell Carlsson, Göran Manneberg, and Peter Unsbo);  
Post-docs 2; Ph.D. students 10

### Summary of Activities

The group is active in cross-disciplinary applied physics based on X-rays, optics, and acoustics. Their major targets are applications in biology and medicine, and, as a spin-off, EUV technology. The most important field of research is X-ray science and technology. Here, a new high-brightness liquid-jet-target laser-plasma source has been developed. By combining this source with novel X-ray optics, they recently demonstrated the first sub-visible-resolution compact X-ray microscope. Such microscopes show promise for cell biological studies where high resolution is important. Furthermore, another version of the liquid-jet source was developed for EUV (Extreme Ultraviolet) projection lithography systems, for future production of integrated circuits with very narrow line widths. In a new project, they demonstrate high-brightness hard X-ray generation with a liquid-metal-jet anode electron-impact source. In addition to the X-ray science and technology, optical and acoustical methods for biomedical applications are investigated.

**University:** KTH  
**Division:** Condensed Matter Physics  
**Head or representative:** Alexander Grishin  
**Group composition (2004):** Faculty 5 (Magnus Andersson, Alexander Grishin, Sören Kahl, Sergey Khartsev, and Östen Rapp); Post-docs 0; Ph.D. students 8

### Summary of Activities

The research activities are concentrated on three main subjects: new functional materials, high- $T_c$  superconductors (HTSC), and metal-insulator transition in quasi-crystals. The group focuses on four types of functional materials: films of MnAs, garnets and manganese oxides; novel ferroelectric films; and iron garnet structures. These materials offer the challenge of combining properties such as superconductivity, ferromagnetism, ferro-electricity, optical transparency, colossal magnetoresistance, etc. In functional materials, several demonstrators have been fabricated spanning a great diversity of applications (modulators, visualisers, bolometers, microsensors, memory cells, varactors, etc.) The work on HTSC is related to the vortex dynamics near the glass transition, the liquid vortex phase, and superconducting fluctuations. The electronic properties of quasi crystals are studied in various samples under different conditions (e.g., irradiation with neutrons).

**University:** KTH  
**Division:** Condensed Matter Theory  
**Head or representative:** Anders Rosengren  
**Group composition (2004):** Faculty 7 (Anders Rosengren, Mats Wallin, Patrick Henelius, Jack Lidmar, Per-Håkan Lundow, Anatoly Belonoshko, and Miklos Gulacsi); Post-docs 2; Ph.D. students 4

### Summary of Activities

Members of this group have many foreign collaborators. They sometimes collaborate with each other and sometimes work with their external collaborators. Much of their work is based on numerical methods, including Monte Carlo and Density Matrix Renormalisation Group. They are tackling a large range of theoretical problems: ranging from random quantum spin chains; to a conjecture on  $T_c$  for the three-dimensional Ising model; to

glass phases in vortex lattices; to corrosion and shock waves in deuterium. They have also been involved in biologically motivated problems, including buckling of viruses and molecular motors (the latter in collaboration with researchers at the Karolinska Institute).

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University: SU  
 Division: Fields and Particles  
 Head or representative: Hans Hansson  
 Group composition (2004): Faculty 2 (Hans Hansson and Anders Karlhede);  
 Post-docs 0; Ph.D. students 4

### Summary of Activities

The group members collaborate with various foreign researchers, and they have also collaborated with other Swedish CMT groups at KTH and GU. The research methods are primarily analytical/field theoretic ones. The group has recently made progress on the  $\nu=1/2$  quantum Hall state, showing that the model on a thin torus is equivalent to free fermions. They believe that it may be possible to show that this state evolves continuously into a one-dimensional Luttinger liquid ground state as the width of the system is increased to infinity, so that the system becomes two-dimensional. They have also recently collaborated with David Haviland, an experimentalist at SU working on nanostructure physics on a model of a qubit.

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University: SU  
 Division: Inorganic Chemistry  
 Head or representative: Osamu Terasaki  
 Group composition (2004): Faculty 7 (Sven Lidin, Osamu Terasaki, Mats Johnsson, Ulrich Häussermann, Kjell Jansson, Tetsu Ohsuna, and Yasuhiro Sakamoto);  
 Post-docs 0; Ph.D. students 13

### Summary of Activities

The activities of Osamu Terasaki's group are concentrated on using periodic spaces such as cavities or channels of high-quality zeolites. The main purpose is to synthesise new cluster-arrays, which exhibit novel properties based on an electronic interaction among the clusters through the periodic arrangements and the quantum mechanical effects. Various high-purity

and high-quality zeolites from nano to large single crystals have been synthesised, and their three-dimensional and surface structures characterised. Sven Lidin's group deals with the synthesis and characterisation of aperiodically ordered material, primarily intermetallic such as zinc-metal rich rare earth compounds. Other activities deal with the energetic background to the stability of incommensurate superstructure ordering, and a more practical aspect of poorly ordered intermetallics – thermoelectricity. Mats Johansson's main research activities consider the synthesis and characterisation of new low-dimensional materials and sintering of structural- and functional ceramics.

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**University:** KTH  
**Division:** Laboratory of Photonics and Microwave Engineering  
**Head or representative:** Ulf Ekenberg (Spintronics group)  
**Group composition (2004):** Faculty 1 (Ulf Ekenberg);  
 Post-docs 1; Ph.D. students 0

#### Summary of Activities

For several years, Ekenberg has been studying band-splitting due to spin-orbit coupling, associated with the Rashba effect. This area is potentially important for the proposed Data-Das spin transistor, which involves rotating the spin of an electron in a semi-conductor channel at a rate controlled by an electric field. With his post-doc, he has studied a model for several III-V semiconductors, which includes conduction, heavy hole, light hole and split-off bands. They tentatively concluded that the Rashba effect is much larger for holes than for electrons. The splitting depends on wave-vector in a much different way for holes than for electrons, and exhibits a large peak at a particular wave-vector associated with an anti-crossing of heavy and light hole subbands. Ekenberg anticipates that his theoretical predictions will be tested by an experimental group that he is associated with at KTH.

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**University:** KTH  
**Division:** Materials Chemistry  
**Head or representative:** Mamoun Muhammed  
**Group composition (2004):** Faculty 4 (Eva Björkman, Mamoun Muhammed, Andrei Zagorodni, and Yu Zhang);  
 Post-docs 2; Ph.D. students 6

### Summary of Activities

The main activities involve the fabrication and processing of nanoparticles and nanomaterials using chemical methods. The materials studied cover a wide range of compositions including metallic, ceramics, intermetallic, semiconductors, composites, and polymeric materials. The group also used thermodynamic modelling for the design of the synthetic route. The activities are diverse and concern the fabrication and study of nanostructured hard materials (WC-Co), superconductors, ZnO, multi-functional nanoparticles, thermoelectric materials, metal oxide catalysts, magnetic nanoparticles, inorganic – organic nanocomposites, nanowires, nanotubes and nanorods, self-assembled nanostructures, etc.

**University:** KTH  
**Division:** Materials Physics, Lab of Materials and Semiconductor Physics  
**Head or representative:** Ulf Karlsson  
**Group composition (2004):** Faculty 10 (Ulf Karlsson, Mats Göthelid, Oscar Tjernberg, Torbjörn Åkermark, Margareta Linnarsson, Nils Nordell, Shi-Li Zhang, Birger Emmoth, Sang-Ho Yun, and Sebastian Lourduoss); Post-docs 2; Ph.D. students 9

### Summary of Activities

This is large group with quite a very wide range of activities, which includes investigations of adsorbates and ultra-thin films on semiconductor and metal surfaces, the electronic structure of bulk oxides (including oxide superconductors), doping and growth of complex semiconductors, and fabrication of model devices exploiting Si-based nanowires and carbon nanotubes. The group is major users of photoemission at MAX-lab, and they have been responsible for the development of a beamline, which is available to the Swedish user community (and others). They have also exploited novel laboratory-based two-photon pump-probe photoemission to investigate the dynamics of excited states at semiconductor surface; and have recently exploited photoemission for bandmapping of the electronic structure of bulk solids, notably of oxide surfaces. A novel variant of this band mapping has been achieved using higher photon energies at the ESRF in Grenoble, offering the ability to achieve “one-shot” band mapping, because at high energies the 2D detector of the Scienta analyser covers the whole Brillouin zone. Other aspects of the surface studies include investigations of model catalytic systems involving complex molecules on

metal surfaces, and the ongoing programme of semiconductor (III-V) surface investigations, including STM imaging supported by a theoretical collaboration. A quite different aspect of the semiconductor work of this group is the major effort invested in the operation of advanced device fabrication and growth facilities in the Electrum Laboratory, at KTH/Kista, which is bearing fruit particularly in the area of MOVPE growth of simple and complex nitrides, and in the fabrication of devices based on silicon and silicide nanowires.

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University: KTH  
 Division: NADA  
 Head or representative: Mikhail Dzugutov  
 Group composition (2004): Faculty 1 (Mikhail Dzugutov);  
 Post-docs 0; Ph.D. students 2

#### Summary of Activities

Dzugutov's research is in understanding fundamental properties of liquids and amorphous solids using classical molecular dynamics simulations with pairwise interatomic potentials. Earlier work showed that cooling of a mono-atomic liquid in a spherically symmetric pair potential environment can lead to the formation of a dodecagonal quasi-crystal, which sustains a high rate of phason flips. Similarly, simulations of super-cooled liquids related the stretched exponential for of relaxation to vacancy-assisted hopping diffusion. On the puzzling issue of the vibrational dynamics of glassy systems, Dzugutov's group was able to relate the dynamics to the local icosahedral order. More recent work (2002) shows that the anomalous behaviour in supercooled liquids approaching the glass transition, results from the formation of low- dimensional clusters.

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University: KTH  
 Division: Nanostructure Physics  
 Head or representative: David B. Haviland  
 Group composition (2004): Faculty 2 (David Haviland and Vladislav Korenivski);  
 Post-docs 1; Ph.D. students 5

#### Summary of Activities

The research activities are focused on three topical subjects: quantum circuits with nanoscale Josephson junctions; spin-dependant transport in nanomagnetic circuits; and nanobiotechnology. The Josephson junction work aims

to understand electronic transport when the superconducting condensate is measured in a situation where the number (not the phase) is a well-defined variable. One-dimensional SQUID arrays are very useful in this regard. The group also performed quantum control experiments using superconducting nanocircuits. The main interest of the spin-dependant transport programme is device concepts and individual nanoscale spin systems, as opposed to thin film production and characterisation. The nanobiotechnology studies are focused on self-assembly as a route to controlled nanofabrication.

**University:** SU  
**Division:** Quantum Chemistry  
**Head or representative:** Anders Nilsson  
**Group composition (2004):** Faculty 4 (Anders Nilsson, Mats Nyberg, Michael Odelius, and Lars G. M. Pettersson);  
 Post-docs 1; Ph.D. students 8

### Summary of Activities

This is a relatively new group headed by Anders Nilsson, who was at Uppsala University for many years, but has recently moved to Stanford, with a part-time position at SU. The group exploits a powerful combination of density functional theory calculations and synchrotron radiation soft X-ray spectroscopies (photoelectron, absorption and X-ray emission – including resonant Raman scattering) to explore the nature of chemical bonding at, or near, surfaces. Recent work concerns the structure and bonding of liquid water. The associated experimental programme involves instrumental developments, with a focus on the use of SSRL at Stanford. Future plans include the completion of a new generation differentially-pumped spectrometer system to allow studies at even higher local pressures, and ambitious ideas to exploit the X-ray free-electron laser facility to be constructed at SSRL.

### LINKÖPING UNIVERSITY

**University:** LiU  
**Division:** Applied Optics  
**Head or representative:** Hans Arwin  
**Group composition (2004):** Faculty 3 (Hans Arwin, Klas Broo, and Kenneth Järrendahl);  
 Post-docs 1; Ph.D. students 2

### Summary of Activities

The research activity is devoted to development and utilisation of ellipsometry for studying the optical properties of materials and thin films. Ellipsometry in combination with modelling is a powerful tool for studying the optical properties of more complex systems. The group has demonstrated these capabilities through their studies of different systems, such as porous Si and SiC. At Linköping University, the ellipsometry activity has a particular good environment, since, among others, there are activities directed towards thin film technology, conducting thin films, multi-layering in life science and nanotechnology and sensor development, in which understanding of the optical properties is essential. Availability of appropriate sample material, which can be found in Linköping, is important. The future plans of the group include participation in development of ellipsometry in the X-ray region.

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<b>University:</b>	LiU
<b>Division:</b>	Applied Physics and Sensor Science and Molecular Physics
<b>Head or representative:</b>	Ingemar Lundström
<b>Group composition (2004):</b>	Faculty 15 (Ingemar Lundström, Bo Liedberg, Pentti Tengvall, Anita Lloyd Spetz, Kajsa Uvdal, Fredrik Winquist, Stefan Klintström, Ragnar Erlandsson, Daniel Filippini, Mats Eriksson, Fredrik Björefors, Tomas Ederth, Tina Krantz-Rülcker, Lars-Gunnar Ekedahl, and Robert Bjorklund); Post-docs 3; Ph.D. students 15

### Summary of Activities

The research within the Division of Applied Physics can be summarised as work on: biomaterials and surface biology; biological nanosystems; catalytic reactions; chemical- and biosensors; scanning probe microscopy; imaging optical methods; RGB-physics and computer screens as versatile light sources; and sensor systems. The division hosts a centre of excellence, Swedish Sensor Centre, S-SENCE (a centre for bio- and chemical sensor science and technology). Ongoing research projects are related to hydrogen detection mechanisms at metal-insulator interfaces, ammonia sensitivity of discontinuous catalytic metal films, field effect devices in silicon carbide for chemical sensing at high temperatures, etc. The division of Sensor Science

and Molecular Physics conducts fundamental and applied work in two closely related fields of biologically inspired science and technology: biosensing and biochip technology, and molecular physics and spectroscopy. Activities are centred on patterning and functionalisation of biochips for optical imaging, molecular design, synthesis, self-assembly and biomimetics, etc.

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**University:** LiU  
**Division:** Biomolecular and organic electronics  
**Head or representative:** Olle Inganäs  
**Group composition (2004):** Faculty 3 (Olle Inganäs, Stefan Welin Klintström, and Fengling Zhang);  
 Post-docs 1; Ph.D. students 10

### Summary of Activities

The research activity of the group is focused on electronically and ionically conducting organic solids, mostly conjugated polymers. They do investigations of polymer physics, polymer optics, and electronics devices (lasers, diodes, LEDs, photodiodes, and solar cells), as well as polymer patterning and processing, in close collaboration with synthetic polymer chemistry groups. They spent effort on the optical optimisation of these thin film devices – sometimes thinner than the wavelength of light absorbed. The methods used include electronic transport and electrochemical measurements, device characterisation, polymer microscopy and transmission spectroscopy, photoluminescence and electroluminescence spectroscopy, spectroscopic ellipsometry, surface energy, and surface plasmon resonance. A growing part of the activity is devoted to biomolecular aspects of organic electronics, as demonstrated in the hybrid materials formed from synthetic conjugated polyelectrolytes; and natural biological polyelectrolytes (such as DNA and proteins). The group is part of the Center of Organic Electronics (COE), financed by the SSF, and is co-ordinator of the Center.

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**University:** LiU  
**Division:** Materials Science Division  
**Head or representative:** Bo Monemar  
**Group composition (2004):** Faculty 18 (Peter Bergman, Irina Buyanova, Weimin Chen, Ragnar Erlandsson, Anne Henry, Per Olof Holtz, Erik Janzén, Leif Johansson, Ulf Lindefelt, Bo Monemar, Wei Xin Ni, Lisa Porter, Galyna

Rudko, Staffan Rudner, Son Nguyen Tien, Qamarul Wahab, Helge Weman, and Rositza Yakimova);  
Post-docs 3; Ph.D. students 19

### Summary of Activities

The research of this very large group is concentrated on the study of wide bandgap semiconductors, including growth and a variety of physical properties. The diversity of the activities is substantial; and only a brief summary can be given. Important activities are the studies of growth and material properties of III-nitride layers and superlattices. Two growth systems (HVPE and MOCVD) for GaN have been optimised. The development on the growth of SiC and the study of the fundamental properties has been continued. Basic studies of dilute III-V nitrides and related heterostructures have been performed. The research activities on spintronics semiconductors and nanostructures include growth and optimisation of artificial materials. Spectroscopic tools investigate quantum dot/wire structures based on different materials systems. A number of novel V-groove quantum wire devices made by self-ordering during MOVPE growth have been studied.

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University:	Campus Norrköping
Division:	Mesoscopic Physics and Nanoelectronics
Head or representative:	Igor Zozoulenko
Group Composition (2004):	Faculty 1 (Igor Zozoulenko); Post-docs 0, Ph.D. Students 2

### Summary of Activities

Zozoulenko achieved a number of grants recently, including two together with an experimentalist in Canada, but all grants are now finished. He mainly works on trajectories and wave functions of non-interacting electrons in confined structures: quantum dots, multi-quantum dots, etc. One-publication reports transport experiments and theory on a square dot. It uses Landauer-Buttiker theory; and what appear to be simple solutions of the single particle quantum mechanics of scattering off a square potential. Zozoulenko has apparently continued such collaboration with (different) experimentalists on similar problems. He seems to have carved a niche for himself, doing calculations involving non-interacting electrons in various

geometries. He collaborates with at least three different experimental groups, in different countries, in this area.

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University: Campus Norrköping  
Division: Organic Physics  
Head or representative: Mats Fahlman  
Group composition (2004): Faculty 1 (Mats Fahlman);  
Post-docs 2; Ph.D. students 2

#### Summary of Activities

The group leader, coming from the Surface Physics and Chemistry group at Linköping University, has recently established his own research activity at the Norrköping Campus. The research interests are close to those of the Surface Physics and Chemistry group, but, in addition, the group has taken up new topics. The research activities include charge transfer across metal – organic and organic – organic interfaces, fabrication and fundamental studies of thin film organic-based magnets, development of polymer light emitting display devices, and hybrid conducting polymer – dye sensitised solar cells. Fabrication and fundamental studies of thin film organic-based magnets is a new direction in the group.

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University: LiU  
Division: Scanning Probe Microscopy  
Head or representative: Ragnar Erlandsson  
Group composition (2004): Faculty 1 (Ragnar Erlandsson);  
Post-docs 0; Ph.D. students 0

#### Summary of Activities

After participating in pioneering work at IBM Almaden Research Center (Silicon Valley, USA), Erlandsson returned to Sweden and chose to build AFM/STM laboratory from scratch in Linköping. With the home-made system his group was able to obtain true atomic resolution and show for the first time in their investigation of the  $7 \times 7$  reconstruction of Si(111) the contrasts effects among similar atoms on the surface. His group also developed the force feedback system, which allows the measurement of tip-sample forces with extreme sensitivity.

**University:** LiU  
**Division:** Surface and Semiconductor Physics  
**Head or representative:** Roger Uhrberg  
**Group composition (2004):** Faculty 3 (Göran Hansson, Roger Uhrberg, and Wei-Xin Ni)  
Post-docs 4; Ph.D. students 5

### Summary of Activities

This group has activities in both semiconductor surface and interfaces and in more mainstream (bulk) semiconductor physics. In the former area, the focus is on the electronic and geometrical structure of Si surfaces and adsorbate layers on them, exploiting core and valence level photoemission (notably at MAX-lab), but also STM complemented by theoretical simulations based on external collaboration. The latter area involves investigation of the growth of Si/Si-Ge materials and heterostructures with various dopants (including ER and Sn) and their electronic and optical properties. A combined MBE/STM system is also being used to investigate a number of quite different growth systems.

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**University:** LiU  
**Division:** Surface Physics and Chemistry  
**Head or representative:** W.R. Salaneck  
**Group composition (2004):** Faculty 4 (W.R. Salaneck, Rainer Friedlein, Michel de Jong, and Xavier Crispin);  
Post-docs 1; Ph.D. students 2

### Summary of Activities

This group is concerned with the electronic structure of conducting polymers and their application in electronic devices. The core technique is ultraviolet photoemission, particularly using specialised laboratory-based instruments, but also exploiting MAX-lab for resonant photoemission. Because of the considerable applications of this work, the group attracts substantial funds from other sources, both industry and the European Commission; the Research Council is providing underpinning funding for the more fundamental physics aspects of the work.

**University:** LiU  
**Division:** Theory and Modelling  
**Head or representative:** Igor Abrikosov  
**Group composition (2004):** Faculty 12 (Igor Abrikosov, Karl-Fredrik Berggren, Bruno Lindqvist, Mathias Boström, Magnus Johansson, Peter Münger, Rolf Riklund, Bo Sernelius, Sergei Simak, Sven Stafström, Chirita Valeriu, and Irina Yakimenko); Post-docs 2; Ph.D. students 14

### Summary of Activities

The Theory and Modelling Group led by Abrikosov is still in its transitory stage because of the recent change of leadership. Abrikosov uses *ab initio* electronic structure calculations. Present work in Abrikosov's group includes extension of *ab initio* calculations to surfaces, nanostructures, and random alloys. The work carried out by others include examination of quantum transport in low-dimensional systems and chaos by Berggren, non-linear dynamical lattice models by Johansson, transport in Au nanowires by Simak, work of Sernelius on Cassimir and van der Waals forces between real metal plates, as well as on surface modes in physics. Sernelius is studying the effect of the radiation from cellular phones, which may lead to attractive forces between blood cells. Riklund has been involved in calculations of non-linear phenomena for anharmonic lattices. Muenger's work on cluster diffusion using MD and DFT led to the prediction of repetition mode (snake-like) of diffusion of Pt heptamers on Pt(111). Joint work with experimental group at Linköping verified his theoretical model. Sven Stafström heads the Computational Physics group at Linköping, and he also serves as the director of NSC (computer center in partnership with Saab).

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**University:** LiU  
**Division:** Thin Film Physics  
**Head or representative:** Lars Hultman  
**Group composition (2004):** Faculty 7 (Lars Hultman, Ulf Helmersson, Jens Birch, Valeriu Chirita Hans Högborg, Jochen Scheider, and Per Persson); Post-docs 5; Ph.D. students 16

### Summary of Activities

The division, founded in the early 1980's, and expanded by the current group, has a mixture of researchers, research subjects, characterisation instrumentation, and materials synthesis equipment. Most of the work involves the study of materials of considerable complexity with a strong applied oriented goal. The main activities are related to the development of new materials, the design of thin films at a nanostructures level, and the evaluation of new synthesis processes. Characterisation as well as computation modelling and simulations are employed with a whole battery of research tools. The materials studied are respectively: hard and functional oxides, semiconductors, nanostructures, and tribological systems. Some of the most significant contributions are growth and study of InAlN epitaxially films, development of new class of TiSiC phases, study of fullerene-like carbon nitride films, molecular dynamics simulation of enhanced cluster mobility, etc. The group is active in a great diversity of topics, mainly directed towards the production of new classes of thin films with high hardness and low friction.

### LUND UNIVERSITY

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University: LU  
Division: Atomic Physics  
Head or representative: Stefan Kröll  
Group composition (2004): Faculty 2 (Stefan Kröll and R.Krishna Mohan Rupavatharam);  
Postdocs 0; Ph.D. students 3

### Summary of Activities

The activities since 2000 are centred on the experimental study of rare-earth-ion-doped (REID) inorganic crystals as possible candidates for quantum computer hardware; and to demonstrate simple quantum gates in such crystals. The scientific activities are divided in three main subjects, all related to quantum phenomena: computing, optics and state storage.

The group recently proposed schemes respectively for i) viable quantum computing in a solid material; ii) single and few photon quantum memories. They also demonstrated techniques for an efficient state-to-state transfer and spectroscopic engineering in REID.

**University:** LU  
**Division:** Chemical Surface Physics  
**Head or representative:** Per Uvdal  
**Group composition (2004):** Faculty 1 (Per Uvdal);  
Post-docs 0; Ph.D. students 2

### Summary of Activities

This small group has activities focused in the area of infrared spectroscopy and spectromicroscopy. The main activity is reflection absorption infrared spectroscopy (RAIRS) of molecular vibrations at surfaces with high sensitivity and resolution, combined with theoretical calculations to simulate not only the observed frequencies (including overtone and combination bands) but also the amplitudes. Future plans include extending the work to the far IR using MAX I. Other work on IR spectromicroscopy using MAX-lab is likely to prove of relevance, particularly to the life sciences community.

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**University:** LU  
**Division:** Materials Chemistry  
**Head or representative:** Reine Wallenberg  
**Group composition (2004):** Faculty 1 (Reine Wallenberg);  
Post-docs 0; Ph.D. students 3

### Summary of Activities

The research on fuel cell materials focuses on novel nanostructured materials and methods for energy conversion, including hydrogen generation and hydrogen utilisation in fuel cells, as well as solving problems by using natural gas and hydrocarbons as feedstock. The nanowire activity is concentrated on field emission of electrons from the tip of carbon nanotubes for, e.g., low-energy illumination, and as extremely coherent and bright electron sources. Using size-selected aerosol or chemically produced clusters as catalytic seed for semiconductor whisker growth, single-phase whiskers, and heterostructures have been produced. A functional device, (a resonant tunneling diode) was built by heterostructures within a whisker.

**University:** LU  
**Division:** Mathematical Physics  
**Head or representative:** Stephanie Reimann  
**Group Composition (2004):** Faculty 2 (Thomas Guhr and Stephanie Reimann);  
 Post-docs 3; Ph.D. students 2

### Summary of Activities

Thomas Guhr and Stephanie Reimann appear to work independently. They are part of a larger theoretical physics group, which also covers other areas of theory besides condensed matter, and indeed Reimann's work on quantum dots has a nuclear theory flavour. Reimann works on the ground state properties of electrons in ideal quantum dots, and arrays of quantum dots and the related problem of cold atoms in optical lattices. The methods used are exact diagonalisation, configuration interaction, and density functional theory. She has ongoing collaborations with groups in Finland, Denmark, and Germany. She and her collaborators have obtained a number of results on the ground state of finite systems. So far, there seems to have been little direct contact of her work with experiment. Guhr does research in a number of different fields, and only a part of his research is really in condensed matter theory. A major interest of his is classical chaos. He has collaborated with experimentalists on a study of the acoustic resonances of aluminium blocks, showing that they obey either Poisson or Gaussian orthogonal ensemble statistics depending on the block shape. He wishes to extend his research to the study of mechanical properties of nanostructures. Both Guhr and Reimann are hoping to develop collaborations with the experimental groups in Lund of Kröll (atomic physics) and Samuelson (Solid State Physics) working on nanostructures.

**University:** LU  
**Division:** Solid State Physics  
**Head or representative:** Lars Samuelson  
**Group composition (2004):** Faculty 17 (Knut Deppert, Gunter Grossman, Anders Gustafsson, Dan Hessman, Mikael Johansson, Lennart Lindström, Lars Montelius, Mats-Erik Pistol, Lars Samuelson, Werner Seifert, Jonas Tegenfeldt, Lars-Erik Wernersson, Hongqi Xu, Jonas Ohlsson, Martin Magnusson, Hongxing Xu, and Pär Omling);  
 Post-docs 6; Ph.D. students 22

### Summary of Activities

The “present” orientation of the research was initiated in 1988, when Lars Samuelson returned to Lund and the Nanometer Laboratory and other central nanofacilities were created. The basic science subjects studied are i) quantum devices based on designed nanoparticles; ii) self-assembled quantum dots; iii) advanced epitaxy for device applications; iv) designed quantum systems for ratchets; v) nanotechnology, nano-structures and life sciences; and vi) nano wires. The main goals are to optimise the interplay between innovative materials science and the opportunities in the fields of quantum physics, to develop futuristic nanoelectronic/photonic devices and new nanodevices for life sciences. They pioneered the use of aerosol techniques for the formation of highly ideal metallic and semiconductor nanoparticles; developed a method of self-assembly of quantum dots; improved the epitaxial growth of hetero-structures; studied tunnelling ratchets; further developed the nanoimprint lithography; demonstrate size- and site controlled formation of nanowires, etc.

University: LU  
 Division: Solid State Theory  
 Head or representative: Koung-An Chao  
 Group composition (2004): Faculty 4 (Carl-Olof Almbladh, Ulf von Barth, Koung-An Chao, and Peter Samuelson);  
 Post-docs 1; Ph.D. students 3

### Summary of Activities

Almbladh and von Barth are many-body theorists active in self-consistent GW calculations, in particular for transition metals and their oxides. They have also carried out fundamental developments in the methodology for calculations of total energy, as well as, response functions using variational functionals within time-dependent density functional theory. Their work goes beyond density functional theory and is geared towards treating excited states and dielectric responses that are beyond the scope of DFT. Their present work targets calculations of linear and non-linear response functions and excitonic effects in optical spectra of nanoscale systems. They also use many-body perturbation techniques to calculate excitation energies of strongly correlated systems, and work closely with experimentalists in the interpretation of data from optical and X-ray spectroscopies. Koung-An Chao’s work is in three major research projects: physics and devices in the terahertz frequency range, the solid-state power generation and refrigeration with energy recycle, and the dynamics of spin-polarised phenomena.

**University:** LU  
**Division:** Synchrotron Radiation Research  
**Head or representative:** Jesper N. Andersson  
**Group composition (2004):** Faculty 5 (Jesper N. Andersen, Ingolf Lindau, Edvin Lundgren, Anders Mikkelsen, and Ralf Nyholm);  
 Post-docs 0; Ph.D. students 5

### Summary of Activities

This group plays a major role in developing the instrumentation, which serves the user community of MAX-lab, but also has two important strands to its own research programme in condensed matter physics. The first of these is concerned with surface science studies of adsorption and reactions at surfaces, especially chemical shifts in high-resolution core-level photoemission to extract information on adsorption sites, but more recently combined with quantitative structural studies using surface X-ray diffraction (obtained at the ESRF and ANKA) and, recently, STM studies. A focus of the “high-pressure” XRD structural studies is oxide formation. Secondly, the group has been applying STM to studies of the internal structure of semiconductor materials using cross-sectional STM of semiconductor nanostructures as a complement to TEM studies of materials grown in the group of Lars Samuelson at Lund University.

## UMEÅ UNIVERSITY AND OTHER SMALL UNIVERSITIES

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**University:** UmU  
**Division:** Experimental Physics  
**Head or representative:** Bertil Sundqvist  
**Group composition (2004):** Faculty 5 (Ove Andersson, Anders Ferry, Tatiana Makarova, Bertil Sundqvist, and Ludvig Edman);  
 Post-docs 3; Ph.D. students 7

### Summary of Activities

The present scientific activity has grown from the research in condensed matter physics started in 1970 and specialising in studies of matter under extreme conditions, e.g., very high pressures. Working under those conditions significantly increases the experimental difficulties, but enables to obtain additional information from the systems studied. Today, the scientific activities shifted; from the use of extreme pressures as such, to the study of new and

interesting materials and their properties. The research of the group can be summarised in three topics: carbon nanostructures, liquid and amorphous solid water, and ion conduction in solid materials. Highlights in the past activities are polymerisation of single crystal  $C_{60}$  into both one- and two-dimensional phases; unexpected discovery of ferromagnetism in  $C_{60}$ ; and electrical transport properties of carbon nanotubes under high pressure.

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University: Kalmar  
 Division: Condensed Matter Physics  
 Head or representative: Carlo M. Canali  
 Group composition (2004): Faculty 1 (Carlo M. Canali);  
 Post-docs 0; Ph.D. students 2

### Summary of Activities

Carlo Canali has started a new degree programme in Kalmar in Nanoscience. His work is in the area of nanomagnetism and spin-dependent transport in magnetic nanoparticles. Motivated by the experiments of magnetic single-electron transistors, Canali has provided interpretation of the experimental results, using simple models for collective magnetisation and quasiparticle degrees of freedom. Canali has also examined the interplay between disorder and Coulomb interaction in mesoscopic systems. He was able to show for the case of interacting electrons in disordered quantum dots that the combined effect of disorder and correlations was that electrons could tunnel into the dot in pairs as the chemical potential was raised. Quantum magnetisation in strongly correlated systems as well as application of the random matrix theory to disordered systems are also among Canali's present work.

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University: Skövde  
 Division: Physics  
 Head or representative: Krister Karlsson  
 Group composition (2004): Faculty 1 (Krister Karlsson);  
 Post-docs 0; Ph.D. students 0

### Summary of Activities

The thrust of the work is in *ab initio* studies of temperature-dependent properties of magnetic materials and semiconductors. This is a challenging area, as popular applications of DFT are confined to 0 K. One of Karlsson's

achievements in recent times is the proposed formalism for calculation of the response function using temperature-dependent Green's function. This has been used to calculate the spectra and dispersion of spin waves ferromagnets, such as Fe and Ni. Furthermore, Karlsson has proposed an exchange-correlation kernel, assuming a local vertex, for usage in time-dependent DFT calculations of the optical absorption spectra of solids.

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**University:** Karlstad  
**Division:** Materials Physics  
**Head or representative:** Lars Johansson  
**Group composition (2004):** Faculty 5 (Lars Johansson, Kjell Magnusson, Ellen Moons, Thijs Holleboom, and Mats Larsson);  
Post-docs 0; Ph.D. students 5

#### Summary of Activities

This is a relatively new group with an active programme, which makes very effective use of synchrotron radiation (at MAX-lab and elsewhere) and of international collaborations. The core activities involve studies of the electronic and geometrical structure of semiconductor surfaces and interfaces (Si and Ge, but also SiC and GaN) and work on self-assembled monolayers of alkane thiols, and more recently other organic films (PTCDA) of potential relevance to electronics applications. The experimental work is complemented by in-house DFT calculations.

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**University:** Luleå  
**Division:** Physics  
**Head or representative:** Hans Weber  
**Group Composition (2004):** Faculty 1 (Hans Weber);  
Post-docs 0; Ph.D. Students 0

#### Summary of Activities

Several of Weber's papers are collaborations with other Swedish physicists on phase transitions involving vortices in superconductors. Collaboration with a group in Germany is on traffic flow, a problem, which is formally related to vortex thermodynamics. Weber's contributions to these projects involve Monte Carlo calculations.

**University:** Mid Sweden  
**Division:** Engineering, Physics and Mathematics  
**Head or representative:** Håkan Olin  
**Group composition (2004):** Faculty 1 (Håkan Olin);  
 Postdocs 0; Ph.D. students 2

### Summary of Activities

The main research activities, in the period of 1997 – 2004, have been experimental studies on nanowires and nanodevices. The most important achievements have been the observation of quantised conductance in Bi nanowires; development of a new instrument combining a tiny STM with a transmission electron microscope; starting a TEM-STM spin-off company; and application of the TEM-STM method to various innovative experiments on nanostructures.

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**University:** Örebro  
**Division:** Solid State Physics  
**Head or representative:** Peter Johansson  
**Group composition (2004):** Faculty 1 (Peter Johansson);  
 Post-docs 0; Ph.D. students 0

### Summary of Activities

Peter Johansson conducts theoretical calculations of the electromagnetic response of nanometer-sized systems by solving classical equations in complex geometries. He has collaborations with several leading experimentalists in the field, and his work facilitates interpretation of experimental data. His theoretical model for calculations of SERS intensities was able to account for the many orders of magnitude enhancement in the Raman scattering cross-section of molecules adsorbed on metallic nanoparticles.

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**University:** Umeå  
**Division:** Theoretical Physics  
**Head or representative:** Jörgen Rammer  
**Group composition (2004):** Faculty 3 (Jörgen Rammer, Peter Olsson, and Andrei Shelankov);  
 Post-docs 1; Ph.D. students 1

### Summary of Activities

This appears to be two completely independent groups: Rammer and Shelankov in one group and Olsson in the other. Rammer and Shelankov are working on a variety of problems in quantum condensed matter theory. Their activities include transport in quantum dots, and they have developed a new approach to the subject based on the “charge projection technique”. Olsson works completely separately on different topics. He has a long-standing collaboration with S. Teitel in the U.S.A. He appears to have formerly been in the group of Petter Minnhagen (his Ph.D. advisor), who recently left Umeå temporarily for NORDITA. Olsson has been working on the classical thermodynamics of vortices in the presence of disorder for many years, using the three-dimensional xy model as a relatively simple starting point. His work is primarily based on Monte Carlo simulations.

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University:	Umeå/NORDITA
“Division”:	NORDITA
Head or representative:	Petter Minnhagen/Kim Sneppen
Group Composition (2004):	Faculty 3 (Petter Minnhagen, Beom Jun Kim, and Kim Sneppen); Post-docs 0, Ph.D. Students 5

### Summary of Activities

This group has had rapid recent changes in its members, activities, and physical location. The senior member, Minnhagen, was at Umeå until 2002, when he accepted a five-year appointment as director of NORDITA (Nordic Institute for Theoretical Physics) in Copenhagen. His research activities were mainly focused on classical critical phenomena, especially in vortex systems, until about 2001, when they moved towards general theory of networks with possible connections to biology, communications, economics, etc. Kim Sneppen has never worked in Sweden for an extended period, as far as we know, but is being funded by the Research Council to do research at NORDITA. His research activities have spanned nuclear physics, general theory of networks, and biophysics. Future plans for both Minnhagen and Sneppen are for research in complex network theory, including biological networks.

## UPPSALA UNIVERSITY

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**University:** UU  
**Division:** Condensed Matter Theory  
**Head or representative:** Börje Johansson  
**Group composition (2004):** Faculty: 7 (Börje Johansson, Rajeev Ahuja, Susanne Mirbt, Sergei Simak, Igor Abrikosov, Lars Nordström, and Natalia Skorodumova);  
 Post-docs 9; Ph.D. students 11

### Summary of Activities

Johansson's work is mainly in the development and application of density functional theory, in order to understand the properties of complex materials. He and his group work very closely with experimentalists, and some of their theoretical methodologies were developed to help analyse experimental data, particularly coming from laboratories at Uppsala University. The group's research activities are centred on; understanding and predicting structural stability, phase transitions, electronic and, in some cases, magnetic properties of advanced materials, such as transition metal oxides, ternary alloys and their complexes, and transplutonium metals. A number of computational tools have been developed by the group: first principles calculations using DFT (full potential LMTO method); *ab initio* lattice dynamics; molecular dynamics using quasi-*ab initio* approach, etc. Group member Ahuja leads the effort in code development, which is expected to be made available for broader dissemination.

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**University:** UU  
**Division:** Condensed Matter Theory  
**Head or representative:** Michael Lieberman  
**Group composition (2004):** Faculty 1 (Michael Lieberman);  
 Post-docs 0; Ph.D. students 2

### Summary of Activities

Lieberman's research covers a broad range of theoretical physics. The aim of the reported work is to increase the theoretical understanding of electronic

and optical properties of the semiconductor nanostructures at high level of excitation of electron-hole pairs, in particular, as a function of external electromagnetic fields. A large variety of semiconductor nanostructures is considered, such as quantum wells (QWS), quantum wires (QWRS) and quantum dots (QDS), and thin films and optical guides. Lieberman investigates the robust, but transient coherence of macroscopic exciton waves in various semiconductor systems. If zero-point energy is comparable or larger than the thermal energy – the effect of the Bose-Einstein statistics become important. He also studies the tunnel-coupled double quantum wires (TCDQW) in a magnetic field, and the behaviour of exciton matter in quantum wires at different densities.

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**University:** UU  
**Division:** Electron Spectroscopy and Molecular Surface Physics  
**Head or representative:** Hans Siegbahn  
**Group composition (2004):** Faculty 3 (Hans Siegbahn, Anders Sandell, and Håkan Rensmo);  
Post-docs 0; Ph.D. students 7

### Summary of Activities

This group is pursuing a broad range of problems involving surface and near-surface phenomena, the common strand being the exploitation of X-ray photoelectron spectroscopy (XPS) and absorption spectroscopy (XAS). Much of this work involves the investigation of systems of considerable complexity, and there is a strong “applied” undercurrent. Most investigations exploit traditional XPS “surface analysis” methods of complex materials science problems, although the use of synchrotron radiation introduces a number of novel aspects. In addition, however, the work also includes more fundamental surface science investigations of well-characterised model surfaces, in some cases chosen to complement the work on the “real systems”. An example of this is the work on dye-sensitised solar cells, complemented by experimental and collaborative theoretical work on the adsorption of the dye molecules on single crystal TiO<sub>2</sub>. Other work, such as that on CVD precursor surface chemistry, focuses on this traditional surface science approach. By contrast, methods much closer to traditional surface analysis are being used to study heparin coating of medical implants to try to improve the biocompatibility of metallic vascular stents.

**University:** UU  
**Division:** Materials Physics  
**Head or representative:** Björgvin Hjörvarsson  
**Group composition (2004):** Faculty 6 (Ola Hartman, Björgvin Hjörvarsson, Tore Ericsson, Roger Wäppling, Bengt Lindgren, and Gabriella Andersson); Post-docs 3; Ph.D. students 6

### Summary of Activities

The principal research activities of this group are focused on magnetism, hydrogen in materials, and energy storage. In magnetism, the relation between finite size and phase transitions is explored. This was accomplished by selective-*in situ* hydrogen doping of magnetic heterostructures. The group also discovered a new class of magnetoresistive semiconductors. The dimensionality aspects of hydrogen in materials have been studied in very thin metallic layers under biaxial strain. This results in a polarisation of the local strain field, generating new phases showing Curie-Weiss fluctuations. The storage of hydrogen in nanosize materials is the main research idea in the field of energy.

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**University:** UU  
**Division:** Neutron Research Laboratory (NFL)  
**Head or representative:** Adrian R. Rennie  
**Group composition (2004):** Faculty 4 (Adrian Rennie, Birger Fogelberg, Robert Delaplane, and Per Zetterstöm); Post-docs 0; Ph.D. students 0

### Summary of Activities

The main role at NFL is to provide facilities for neutron beam research to the Swedish scientific community. It also acts as centre of expertise in neutron techniques for Sweden, and thus acts as a focus for collaboration with other research groups in Sweden and internationally. The wide range of projects includes: structural studies and crystallography (perovskites); diffuse scattering and amorphous materials (glasses and liquids as well as structure of nano-materials and crystals); energy storage materials (metal hydride systems); soft matter and interface work (complex fluids, such as dispersions of particles); and other advanced materials (bimetallic composite materials).

**University:** UU  
**Division:** Soft X-ray Physics  
**Head or representative:** Joseph Nordgren  
**Group composition (2004):** Faculty 6 (Joseph Nordgren, Sergei Butorin, Laurent Duda, Martin Magnuson, Jan-Erik Rubensson, and Lars Werme);  
Post-docs 2; Ph.D. students 6

### Summary of Activities

This group develops and uses soft X-ray spectroscopic techniques to study gaseous, liquid and solid matter, and in particular X-ray emission spectroscopy (XES) and resonant inelastic X-ray scattering (RIXS). These methods are being applied to fundamental and applied aspects of strongly correlated systems, to the molecular structure of liquids and solutions; and to investigate the electronic structure of novel materials. A major theme of this group has been instrumental development for these methods. They have built up facilities for these experiments at MAX-lab, which can be accessed by other Swedish groups, as well as at the ALS in the USA. The photon-in/ photon-out character of the method allows it to be applied to a wide range of problems (not constrained by UHV or localised at surfaces). While fundamental electronic structure work forms the core of the activity, the recent work on the problem of nuclear waste dissolution in ground water provides an illustration of its potential for far more applied problems. In this study, the method has been used to establish that Fe is capable of reducing (soluble) higher oxidation states of uranium to insoluble  $U_4^+$ , a conclusion reached as a result of investigating a Fe/aqueous solution interface on the water side of a thin X-ray window.

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**University:** UU  
**Division:** Solid State Physics: Magnetism  
**Head or representative:** Per Nordblad  
**Group composition (2004):** Faculty 3 (Per Nordblad, Peter Svedlindh, and Klas Gunnarsson);  
Post-docs 1; Ph.D. students 7

### Summary of Activities

This group has a very broad range of scientific activities related to magnetic materials and a more focused effort in superconductivity. The topics studied

include disordered and frustrated spin systems, magnetic films and multilayers, nanomagnetism, biomagnetism, diluted magnetic semiconductors, manganese perovskite films, and flux dynamics in superconductors. Most significant contributions are: exploration of the non-equilibrium character of the low temperature spin glass phase; extensive studies of high-quality magnetic superlattices; increase of the Curie temperature by more than 70K during low-temperature annealing of (Ga, Mn)As; confirmation of the magnetic ageing; and memory and rejuvenation effects in Bi-based superconductors.

**University:** UU  
**Division:** Solid State Physics: Material Optics  
**Head or representative:** Claes-Göran Granqvist  
**Group composition (2004):** Faculty 10 (C. G. Granqvist, M. Furlani, P. Heszler, R. Karmhag, L. Kish, G. A. Niklasson, C-G Ribbing, A. Roos, M. Strömme, and E. Wäckelgård);  
 Post-docs 3; Ph.D. students 29

### Summary of Activities

The Division of Solid State Physics is part of the Department of Engineering Sciences, and its research activities range from fundamental aspects of solid-state physics to technological applications. Most senior researchers formally belong to three sections: technology, physics, and chemistry. Electromagnetic properties of materials are the main interest of the research activities. They range from the optical properties of materials, such as photonic bandgap (Ribbing); solar absorbing coatings (Wäckelgård); optical modelling (Niklasson, Roos); over nanomaterial science, such as metal-oxide nanoparticles (Heszler, Niklasson, Granqvist) to technological interesting topics, such as electrochromic materials for “smart windows” (Niklasson, Granqvist) and pharmaceutical materials for “drug delivery” (Strömme).

**University:** UU  
**Division:** Surface Physics  
**Head or representative:** Nils Mårtensson  
**Group composition (2004):** Faculty 5 (Nils Mårtensson, Dimitri Arvanitis, Jonathan Hunter Dunn, Olof Karis, and Carla Puglia);  
 Post-docs 4; Ph.D. students 5

### Summary of Activities

This group plays a major role in the development and support of synchrotron radiation photoemission and absorption spectroscopies at MAX-lab, which benefit the whole Swedish community (and others), and in the past have been involved in instrumentation advances, one of which led to the Scientia hemispherical electron energy analysers. A core activity is in electron spectroscopy including resonant photoemission and the development of the “core-hole clock” technique to probe electron dynamics. Traditional surface science applications, however, are being complemented by studies of increasing complex systems, such as adsorbed dye molecules, porphyrines, and phthalocyanines. A strong component of adsorption studies motivated by traditional heterogeneous catalysis continues. In addition, the implementation of a special facility to allow solution-deposited films into the UHV spectrometers under well-controlled conditions will further broaden this range of applications into important new areas. Recent work on clusters could prove to be a very important new theme for this group. A further important component of this group’s work is concerned with thin film magnetic systems, including magnetic dichroism studies. In addition, a new MAX II beamline based on a variable-polarisation undulator is now being constructed, to make further inroads into this problem. A new exploratory collaborative programme concerns the exploitation of the high coherence of third-generation synchrotron radiation sources, such as MAX II, to investigate magnetic speckle.

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**University:** UU  
**Division:** Theoretical Magnetism  
**Head or representative:** Olle Eriksson  
**Group composition (2004):** Faculty 6 (Olle Eriksson, Lars Nordström, Sergei Simak, I. Sandalov, M.Knatsnelson, and G.Grechnev);  
Post-docs 6; Ph.D. students 12

### Summary of Activities

Eriksson’s group started two years ago. Like Börje Johansson, Eriksson’s work is also in the area of density functional theory with special emphasis on magnetism. His work in the early nineties focused on orbital moments at surfaces and interfaces. More recent work is on magnetic semiconductors, using a combination of first principles calculations and Monte Carlo simulations for predicting characteristics, such as magnetic moments,

conductivity, and critical temperatures for spintronic behaviour. Through a variety of applications of accurate and robust electronic structure calculations to technologically advanced materials, Eriksson and co-workers have established the importance of theoretical and computational studies in understanding and controlling the properties of these materials. Their interest also lies in theoretical studies of magnetic anisotropy energy in alloys and other complex materials using accurate techniques.











**Administrative part**

Co-operation with other research groups, 2001-2004 (that have resulted in co-publications)

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Visits to foreign research groups, 2001-2004 (for longer duration than 1 month)

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**Scientific part**

Description of scientific activity (No more than 3 pages per group)

**Scientific part**

Most significant scientific contribution during the last 5-10 years (No more than 1 page per group)

**Scientific part**

Future plans (No more than 1 page per group)

**Scientific part/Questions to each single grant holder**

<p>Please answer personally to the following three questions (No more than 1/2 page per grant holder):</p> <p>1 Describe, in order of priority, what you consider to be the strength of Swedish Condensed Matter Physics                  2 Describe, in order of priority, what you consider to be the weakness of Swedish Condensed Matter Physics                  3 Other comments</p>
<p>Name:</p> <p>1 2 3</p>

# APPENDIX 4

## Short CVs of the Experts

### Professor Anne Borg

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- Professor of Physics (1998), Department of Physics, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway
  - Born in Drammen, Norway, in 1958;
  - Sivilingeniør (M.Sc.) and Dr.ing (Ph.D.), NTH (currently NTNU), Trondheim, Norway.
- 

#### Special Assignments:

Associate Professor and Professor of Physics, NTNU, Norway (1991–present); Visiting scientist, Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, USA (1998–1999); Scientific advisor, SINTEF Applied Physics (1991–1999, 2002–present); Member of the Norwegian Physical Society (1987–present); Member of the Norwegian Academy of Technical Sciences (NTVA) (2000–present); Member of The Royal Norwegian Academy of Sciences (2002–present); Vice-president of the Norwegian Physical Society (2002–2003); President of the Norwegian Physical Society (2004–present); Member of the IUPAP Working Group on Women in Physics (2004–present); Member, “Forvaltningsutvalget for “Sivilingeniørstudiet”, NTNU (1999–present); Member, Board of the Norwegian Academy of Technical Sciences (2005–present);

Member, Committee on Materials Physics and Chemistry, Norwegian Research Council (1994–1998); Member, “Fagplanutvalg i fysikk”, Norwegian Research Council (2001); Member, “Beredningsgrupp i kondenserade materiens fysik”, Swedish Research Council (2001–2004); Member, Committee on Computational Resources, Norwegian Research Council (2005–present).

#### Special Scientific Interests:

Experimental surface science. Structural, electronic, and optical properties of surfaces and nanoscopic structures. Scanning probe microscopy techniques, photoelectron spectroscopies and optical techniques applied to surfaces and interfaces.

## Professor Yvan Bruynseraede

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- Professor Emeritus of Physics (2003), Laboratory of Solid State Physics and Magnetism, Catholic University of Leuven (KULeuven), B-3001, Heverlee, Belgium
  - Born in Oostende, Belgium, in 1938;
  - M.Sc. and Ph.D. in Physics, KULeuven, Belgium; CERN Postdoctoral and Associate Fellow, Geneva, Switzerland.
- 

### Special Assignments:

Lecturer and Professor of Physics, KULeuven, Belgium (1972–2003); Chairman, Laboratory of Solid State Physics and Magnetism, KULeuven (1993–2003); Chairman, Research Council, KULeuven (1990–1995); Fellow, American Physical Society (1990–present); Member, Editorial Board of *Phys.Rev.* (1991–1997); Member, Council Research Management, KULeuven (1995–present); Chairman, Expert Research Committee, Flemish Inter-university Council VLIR (2000–2003);

Member, Royal Flemish Academy of Belgium for Science and the Arts, KVAB (1988–present); Member, Council of the ESRF, Grenoble, France (1988–1998); Chairman, Belgian Physical Society (1989–1991); Member, Board of the Belgian Nuclear Research Centre SCK.CEN Mol (1991–present); Co-ordinator, Belgian Interuniversity Attraction Pole Programme (1996–present); Member, Board of the European Physical Society, EPS, France (1997–2001); President, KVAB (1999–2000); Member, Board of the Institute for Radioactive Elements, IRE, Belgium (1999–present); Member, European Academy of Sciences and Arts, Vienna, Austria (2001–present); Member, Board of Regents KULeuven (2003–present);

Member, Committee of Solid State Physics, National Fund for Scientific Research, NFWO, Belgium (1984–1994); Member, Committee of National & International Relations, Flemish Council for Science Policy VRWB (1990–1994); Member, Committee of Science Management VRWB (1994–present); Chairman, Scientific Advisory Committee SCK.CEN Mol (1997–present); Member, International Advisory Committee IFIMUP, Portugal (1998–present); Member, Expert to Advisory Committees, VR and SSF, Sweden (2000–present); Member, Reviewing Committee, Grenoble High Magnetic Field Laboratory, GHMFL, France (2002); Member, Expert Advisory Group EU-FP6, Brussels, Belgium (2002–present); Member, Strategic Advisory Committee, Flemish Institute for Technological Research VITO, Belgium (2002–present);

**Special Scientific Interests:**

Experimental Solid State Physics. Electrical, magnetic, and optical properties of mesoscopic and nanoscopic structures; superconducting vortices in thin films; superconducting/magnetic heterostructures; magnetic interactions in thin films and superlattices; X-ray structural analysis; SPM techniques applied to surfaces and interfaces; studies at very low temperatures and high pulsed magnetic fields.

**Professor Talat S. Rahman**

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- University Distinguished Professor (2001), Department of Physics, Cardwell Hall, Kansas State University, Manhattan, Kansas 66506, USA
  - B.Sc., Karachi; M.Phil., Islamabad (Pakistan), Ph.D. Rochester.
- 

**Special Assignments:**

Postdoctoral Fellow (1977–1979); Research Physicist (1979–1982), University of California, Irvine; Assistant Professor (1983–1986), Associate Professor (1986–1991), and Professor (1991–2001), Kansas State University; Visiting University Professor (2000), Helsinki University of Technology; Visiting Scientist, (Summers of 1998, '99, '01, '02, '03, '04, Fritz Haber Institute, Berlin; Visiting Scientist (1997) Max Planck Institut für Strömungsforschung, Göttingen; Visiting Scientist (1996), Free University Berlin; Professor Invité (1993) EPFL, Lausanne; Visiting Physicist (1992–1993), Brookhaven National Laboratory; Visiting Scientist (1992), Sandia Laboratories, Livermore; Guest Scientist (Summer Months of 1984–1989, '91), Forschungszentrum, Jülich; Faculty Research Participant (1990 and 1995), Argonne National Laboratory; Adjunct Professor, National Center for Physics (2004–2009), Quaid-e-Azam University, Pakistan.

Member, Advisory Board (2004–2006), GIK Institute of Technology, Pakistan; Member, Executive Committee (2002–2005), Division of Materials Physics, American Physical Society; Editorial Board Member (2003–present), Journal of Theoretical and Computational Nanoscience; Co-organizer, Annual International Nathiagali Summer College (1998–present); President-Elect (1997–1998), President (1998–1999), Past-President (1999–2000), Faculty Senate, Kansas State University; Director (1997–2000), Center for Scientific Supercomputing, Kansas State University; Distinguished Sigma Xi Lecturer (2004–2006), USA; Advisor, Developing Scholars' Programme, Kansas State University (2000–present).

**Special Scientific Interests:**

Theory and modelling of phenomena at solid surfaces and nanostructures; theoretical determination of structure, vibrational dynamics, thermodynamics, anharmonicity, chemisorption, reactivity, and atomic diffusion at complex solid surfaces; multi-scale modelling of surface phenomena using lattice dynamics, molecular statics and dynamics, *ab initio* electronic structure calculations, and kinetic Monte Carlo techniques; *ab initio* and phenomenological studies of single-molecule magnets.

**Professor Cyrus R. Safinya**

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- Professor of Materials, Physics, and Molecular, Cellular, and Developmental Biology, Materials Research Laboratory, University of California, Santa Barbara CA 93106
  - Born in New York, NY, USA, in 1954;
  - B.Sc. in Physics and Mathematics (Bates College, 1975), Ph.D. in Physics (M.I.T, 1981): Thesis advisor: Robert J. Birgeneau, Chancellor of UC, Berkeley.
- 

**Special Assignments:**

Research Physicist, Senior Physicist, Staff Physicist, and Senior Staff Physicist; Exxon Research & Engineering (1981–1992); Project Leader, X-ray Scattering, Exxon Research & Engineering Co. (1989–1992); Visiting Directeur de Recherche, Curie Institute, (Paris, 1994); Professor, Materials Department, Physics Department, UC, Santa Barbara (1992–present); Professor, Biomolecular Science & Engineering Programme, UC, Santa Barbara (1994–present); Visiting Professor, University of Rome, “La Sapienza”, (2004); Professor, Molecular and Cellular Developmental Biology Department, UC, Santa Barbara (2004–present).

Co-Chair, (with S. Safran and P. Pincus) the first Materials Research Society Symposium on Macromolecular Liquids (later renamed Complex Fluids), (1989); Chair, the first Gordon Research Conference on Complex Fluids (1990); Co-Chair (with P. Pincus), Workshop on Biomolecular Materials (Santa Barbara, August 1994); Co-Coordinator, ITP Programme on “Physics of Biomembranes”, Santa Barbara, CA (1994); Fellow, The American Physical Society (elected 1994); Henri De Rothschild Foundation Fellow (Curie Institute, Paris, 1994); Section Editor, Biomaterials, Current Opinion in Solid State & Materials Science (1995–1997); Fellow, The American Association for the Advancement of Science (elected 1997); Member, Workshop on Scientific Directions at the Advanced Light Source, Lawrence

Berkeley National Laboratory, Berkeley, California, (1998); Chair, Complex Materials Conference in Honor of P. Pincus, Santa Barbara, (1999); Panel Member, National Academy of Sciences-National Research Council Committee on Developing a Federal Materials Facilities Strategy (1999); Editorial Board, Publishing Programme, Molecular & Chemical Sciences, Gordon & Breach, (2000 -); Editorial Board, Molecular Therapy (American Society of Gene Therapy), (2000-2003); Panel Member, External Site Visitor Committee, NSF site visit to the Synchrotron Research Center, University of Wisconsin Madison, Madison WI, (2000); Member, DOE Council on Materials Science, "Macromolecules at Interfaces", Santa Fe (2001); Lead Reviewer for the Ohio Board of Regents, Physics department, Case Western Reserve University, to establish an Endowed Eminent Scholar Chair in Condensed Matter Physics, (2001).

Workshop on the Application of Biology to the Physical & Material Sciences, DOE Office of Basic Energy Sciences, San Diego (2002), [www.sc.doe.gov/bes/besac/BiomolecularMaterialsReport.pdf](http://www.sc.doe.gov/bes/besac/BiomolecularMaterialsReport.pdf); Member, work-shop on the Application of Biology to the Physical & Material Sciences, DOE Office of Basic Energy Sciences, San Diego, (2002); Member, Director's Review Panel of Stanford Synchrotron Radiation Laboratory's Materials and Chemical Science under SPEAR3, Stanford, CA, (2003); Guest Editor, Current Medicinal Chemistry, "Non-viral Vectors for Gene & Drug Delivery" January issue (2004); Chair, External Site Visitor Committee, NSF site visit to review the Synchrotron Research Center, University of Wisconsin Madison, Madison WI, (2004); Member, External Site Visitor Review Committee, DOE site visit to review Condensed Matter Physics, Brookhaven National Laboratories, Upton, NY, (2004); Co-Chair, external Review Committee, Chemical Physics Interdisciplinary Graduate Programme, Kent State University, Kent Ohio, April 2005; Member, International Advisory Board, Soft Matter Composites, EU-Network of Excellence (2005 -).

#### Special Scientific Interests:

Structures and interactions of supramolecular assemblies of biological molecules, soft matter systems, and liquid crystals. Current research is to elucidate the key parameters that control the interactions between proteins derived from the eukaryotic nerve cell cytoskeleton, which lead to hierarchical supramolecular structures on the nanometer to micron scale, understanding DNA interactions with oppositely charged biomolecules as relates to DNA "packing", and on developing synthetic carriers of genes for delivery applications. Author of chapter on Biophysics for Cambridge University Press' 2nd edition of *The New Physics for the Twenty-First Century* (Edited by Gordon Fraser). The combined chapters will span the whole spectrum of modern physics. (ISBN: 0521816009, available from November 2005).

## Professor Hiroyuki Sakaki

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- Professor of Solid State Electronics (1987), Department of Informatics and Electronics, Institute of Industrial Science, University of Tokyo, 4-6-1 Komaba, Meguro-ku, Tokyo 153-8505, Japan
  - Born in Nagoya, Japan, in 1944;
  - M.Sc. and Ph.D. degrees in Electronic Engineering, University of Tokyo (UT), Tokyo, Japan.
- 

### Special Assignments:

Associate Professor at the Institute of Industrial Science (IIS), University of Tokyo (UT) (1973–1987); Visiting scientist, Leo Esaki's group, IBM Watson Research Center, USA (1976–1977); Professor at IIS, UT (1987–present); Co-appointed Professor, Research Center for Advanced Science and Technology, UT (1988–1998); Director, JST's ERATO "Quantum Wave" Project (1988–1993); Principal Investigator, JST's Int'l Collaborative Research Project on Quantum Transitions (1994–1998); Visiting Professor, Ecole Normale Supérieures, France (1999); Vice President, Japan Society of Applied Physics (JSAP) (2002–2004); President, JSAP (2004–2006); Fellow, American Physical Society (2000–present); Fellow, Institute of Electrical and Electronic Engineers (1998–present).

### Special Scientific Interests:

Semiconductor physics and electronics; Quantum control of electrons in nanostructures;

Electronic and photonic properties of low-dimensional (LD) electron systems, including quantum wells (QW's), quantum wires (QWR's), and quantum dots (QD's); Molecular beam epitaxy of semiconductor nanostructures; and manipulations and applications of LD electrons for advanced electronic and photonic devices.

## Professor D. Phillip Woodruff

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- Professor of Physics (1987), Physics Department, University of Warwick, Coventry CV4 7AL, United Kingdom
  - Born in Hyde, UK, in 1944;
  - B.Sc. Bristol, Ph.D. and D.Sc., Warwick, UK.
-

**Special Assignments:**

Research Fellow (1968–1969) Lecturer (1969–1983) Senior Lecturer (1983–1987), Professor (1987–present), Physics Department, University of Warwick.

Consultant, Bell Laboratories, Murray Hill, NJ, USA (1979 and 1981); Visiting scientist, Fritz Haber Institute, West Berlin (1982); Consultant, A.T.& T. Bell Laboratories, Murray Hill, NJ, USA (1985); Scientific Co-ordinator for Design Study of “Daresbury Advanced Photon Source”, Science and Engineering Research Council (1989–1990); EPSRC Senior Research Fellow (1998–2003); Scientific Consultant at Fritz-Haber-Institute, Berlin (1998–2002).

Member, (1974–1978, 1981–1984), Chairman (1975–1977), Thin Films and Surfaces Group, Institute of Physics; Member (1982–2004), Chairman (1985–1990) British Vacuum Council; Member, SERC Synchrotron Radiation Facility Committee, (1985–1990)

Member, SERC Physics Committee & subcommittees (1986–1990); Scientific Secretary (1989–1992), Scientific Director (1992–1995), President Elect (1995–1998), President (1998–2001), Past President (2001–2004) International Union for Vacuum Science, Techniques, Applications (IUVSTA); Member, MAX-Lab Programme Advisory Committee (1992–present); Member, ELETTRA Programme Advisory Committee, Trieste, Italy; Member (1995–1998); Member, Scientific Advisory Committee, European Synchrotron Radiation Facility (ESRF), Grenoble, France (1999–2002); Member (2000–2002), Chairman (2002–2004) DIAMOND Scientific Advisory Committee; Member, Leibniz-Gemeinschaft Evaluation Committee of BESSY (2004)

**Special Scientific Interests:**

Experimental surface science; Quantitative determination of surface structure by electron and ion scattering methods; Synchrotron radiation methods; Chemisorption and surface reactions; Electronic structure of surfaces and ultra-thin films; Application of density-functional theory to surface adsorption; Surface restructuring.

# APPENDIX 5

## List of Acronyms

AFM.....	Atomic Force Microscope
ALS.....	Advanced Light Source
ANKA.....	Angströmquelle Karlsruhe GmbH
APS.....	American Physical Society
ARPES.....	Angle-Resolved Photoemission Spectroscopy
ATP.....	Adenosine Triphosphate
CBE.....	Chemical Beam Epitaxy
CCD.....	Charge-Coupled Device
CERC.....	Combustion Engine Research Centre
CMOS.....	Complementary Metal Oxide Semiconductor
CMP.....	Condensed Matter Physics
CMR.....	Colossal Magnetoresistance
CMT.....	Condensed Matter Theory
CNRS.....	Centre National de la Recherche Scientifique (French National Center for Scientific Research)
CNT.....	Carbon Nano Tube
CPT.....	Cooper Pair Transistor
CTH.....	Chalmers University of Technology
CVD.....	Chemical Vapor Deposition
DFT.....	Density Functional Theory
DLS.....	Dynamic Light Scattering
DMFT.....	Dynamical Mean-Field Theory
DMRG.....	Density Matrix Renormalisation Group
DMS.....	Diluted Magnetic Semiconductor
DNA.....	Deoxyribonucleic Acid
DOPA.....	Dihydroxyphenylalanine
DRAM.....	Dynamic Random Access Memory
DXPS.....	Dichroism X-ray Photoemission Spectroscopy
EC.....	European Commission
ESS.....	European Spallation Source
EMP.....	Experimental Mesoscopic Physics
EPFL.....	École Polytechnique Fédérale de Lausanne (Swiss Federal Institute of Technology)
ESRF.....	European Synchrotron Radiation Facility

EU.....	European Union
EUV.....	Extreme Ultraviolet
FET.....	Field Effect Transistor
FP6.....	The Sixth Framework Programme
FTIR.....	Fourier Transformed Infra-Red
GMR.....	Giant Magnetoresistance
GTP.....	Guanosine Triphosphate
GU.....	Göteborg University
HBT.....	Heterojunction Bipolar Transistor
HEMT.....	High Electron Mobility Transisto
HFET.....	Heterostructure Field Effect Transistor
HiK.....	University of Kalmar
HiS.....	University of Skövde
HOMO/LUMO.....	Highest Occupied Molecular Orbital/ Lowest Unoccupied Molecular Orbital
HREELS.....	High Resolution Electron Energy Loss Spectroscopy
HTSC.....	High-Temperature Superconductor
HVPE.....	Hydride Vapor Phase Epitaxy
IGBT.....	Insulated Gate Bipolar Transistor
ILL.....	Institut Laue-Langevin
INVAR.....	Invariable under heating
IR.....	Infrared
ISBT.....	Intersubband Transition
ISIS (not an acronym).....	Pulsed Neutron and Muon Source Located at the UK Rutherford Appleton Laboratory
IT.....	Information Technology
IUPAP.....	International Union of Pure and Applied Physics
IXS.....	Inelastic X-ray Scattering
JJ.....	Josephson Junction
KaU.....	Karlstad University
KTH.....	Royal Institute of Technology
LD.....	Low-Dimensional
LED.....	Light Emitting Diode
LEED.....	Low-Energy Electron Diffraction
LiU.....	Linköping University
LMTO.....	Linear Muffin-Tin Orbital
LSI.....	Large-Scale Integration
LTH.....	Lund Institute of Technology
LTSC.....	Low-Temperature Superconductor
LTU.....	Luleå University of Technology
LU.....	Lund University

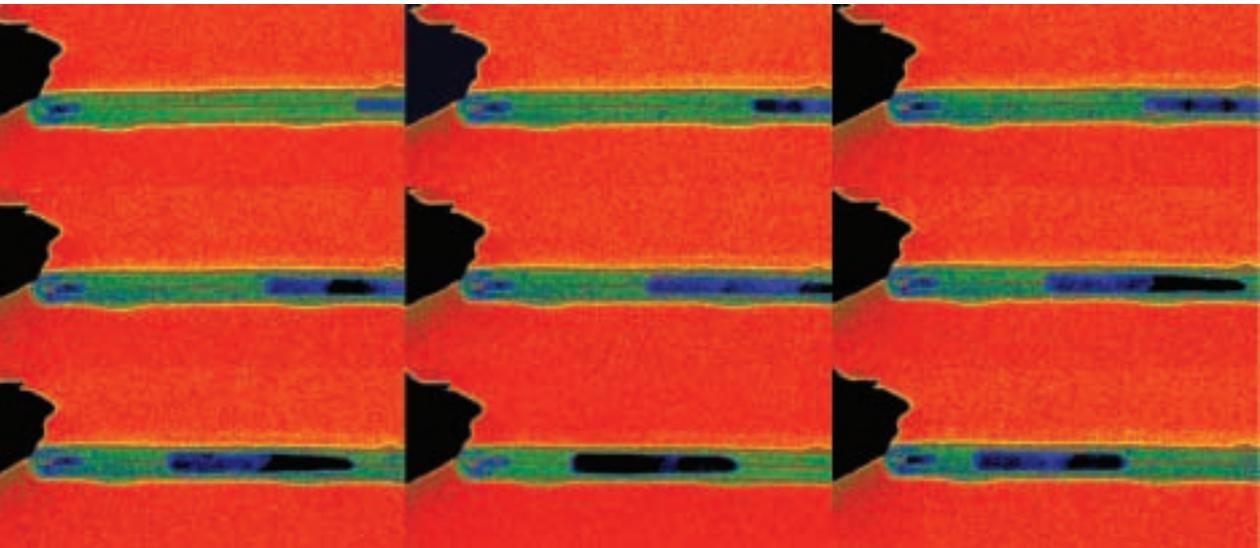
MAX.....	Microtron Accelerator for X-rays
MBE.....	Molecular Beam Epitaxy
MC.....	Monte Carlo
MC2.....	Microtechnology Center
MD.....	Molecular Dynamics
MEM.....	Micro-Electro-Mechanical System
MFM.....	Magnetic Force Microscopy
MH.....	Mid Sweden University
MIR.....	Mid-Infrared
MIS.....	Metal-Insulator-Semiconductor
MOCVD.....	Metal Organic Chemical Vapour Deposition
MOKE.....	Magneto-Optical Kerr Effect
MOS.....	Metal Oxid Semiconductor
MOS-FET.....	Metal Oxide Semiconductor, Field Effect Transistor
MOVPE.....	Metal-Organic Vapour Phase Epitaxy
MRAM.....	Magnetic Random Access Memory
MRI.....	Magnetic Resonance Imaging
MTJ.....	Magnetic Tunnel Junction
$\mu$ SR.....	Muon Spin Rotation
NEM.....	Nano-Electro-Mechanical
NEMS.....	Nanoelectromechanical Systems
NEXAFS.....	Near Edge X-ray Absorption Fine Structure
NFL.....	Studsvik Neutron Research Laboratory
NFR.....	Swedish Natural Science Research Council
NMR.....	Nuclear Magnetic Resonance
NNI.....	Nanoscience and Nanotechnology Initiative
NORDITA.....	Nordic Institute for Theoretical Physics
Nordsync.....	Nordic Consortium for Participation in ESRF
NSC.....	Swedish National Supercomputer Center
NT.....	Council for Natural and Engineering Sciences
NT.....	Semiconducting Nanotube
OLED.....	Organic Light-Emitting Diode
OrU.....	Örebro University
PAQ.....	Phase-Space Absorption Quenching
PDD.....	Photo Dynamic Diagnostics
PDT.....	Photo Dynamic Therapy
PEEM.....	Photo Emission Electron Microscopy
PHOREMOST.....	Nanophotonics to Realize Molecular-Scale Technologies
PLIF.....	Planar Laser Induced Fluorescence
PME.....	Paramagnetic Meissner Effect

PTCDA.....	3,4,9,10-Perylene Tetracarboxylic Dianhydride
PVD.....	Physical Vapour Deposition
QCA.....	Quantum Cellular Automata
QCSE.....	Quantum Confined Stark Effect
QD.....	Quantum Dot
QHE.....	Quantum Hall Effect
QHS.....	Quantum Hall System
QPC.....	Quantum Point Contact
QW.....	Quantum Well
QWIP.....	Quantum Well Infrared Detector
QWR.....	Quantum Wire
R&D.....	Research and Development
RAIRS.....	Reflection Absorption Infrared Spectroscopy
RE.....	Rare-Earth
REID.....	Rare-Earth-Ion-Doped
Review Panel L.....	Semiconductor Physics, Electronics, Electrical Engineering and Photonics
Review Panel O.....	Condensed Matter Physics
Review Panel P.....	Engineering Physics
Review Panel Q.....	Materials Sciences
RF-SET.....	Radio-Frequency Single Electron Transistor
RGB.....	Red-Green-Blue
RIXS.....	Resonant Inelastic X-ray Scattering
RTD.....	Resonant Tunnelling Device
SAM.....	Scanning Electron Microscopy
SAXS.....	Small Angle X-ray Scattering
SEM.....	Scanning Electron Microscopy
SEMPA.....	Scanning Electron Microscopy with Polarisation Analysis
SERS.....	Surface-Enhanced Raman Scattering
SET.....	Single Electron Transistor
SFQ.....	Single Flux Quantum
SIN.....	Superconductor-Insulator-Normal Metal
SL.....	Super Lattice
SNIC.....	Swedish National Infrastructure for Computing
SNN.....	Swedish Nanotechnology Network
SNOM.....	Scanning Near-Field Optical Microscopy
SOI.....	Silicon on Insulator
SP resonance.....	Surface Plasmon Resonance
SPM.....	Scanning Probe Microscopy
SPSTS.....	Spin-Polarised Scanning Tunnelling Spectroscopy

SQUID.....	Superconducting Quantum Interference Device
SRAM.....	Static Random Access Memory
SSF.....	Swedish Foundation for Strategic Research
SSRL.....	Stanford Synchrotron Radiation Laboratory
STEM.....	Sweden Energy Agency
STM.....	Scanning Tunnelling Microscopy
SU.....	Stockholm University
SUNY.....	State University of New York
SXES.....	Soft X-ray Emission Spectroscopy
TCDQW.....	Tunnel-Coupled Double Quantum Wire
TEM.....	Transmission Electron Microscopy
TFR.....	Swedish Research Council for Engineering Sciences
TMR.....	Tunnel Magnetoresistance
TR-XMCD.....	Time-resolved XMCD
TR-XMLD.....	Time-resolved XMLD
UHV.....	Ultra-High Vacuum
UmU.....	Umeå University
UU.....	Uppsala University
UV.....	Ultraviolet
UV-Vis.....	Ultraviolet and Visible Absorption Spectroscopy
vdW.....	van der Waal
VINNOVA.....	Research and Innovation for Sustainable Growth
VPE.....	Vapor Phase Epitaxy
VR.....	Vetenskapsrådet (Swedish Research Council)
XAFS.....	X-ray Absorption Fine-Structure
XAS.....	X-ray Absorption Spectroscopy
XES.....	X-ray emission spectroscopy
XMCD.....	X-ray Magnetic Circular Dichroism
XMLD.....	X-ray Magnetic Linear Dichroism
XPS.....	X-ray Photoelectron Spectroscopy
XRD.....	X-ray Diffraction
XRMS.....	X-ray Resonant Magnetic Scattering
XSTM.....	Cross-Sectional Scanning Tunnelling Microscopy

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