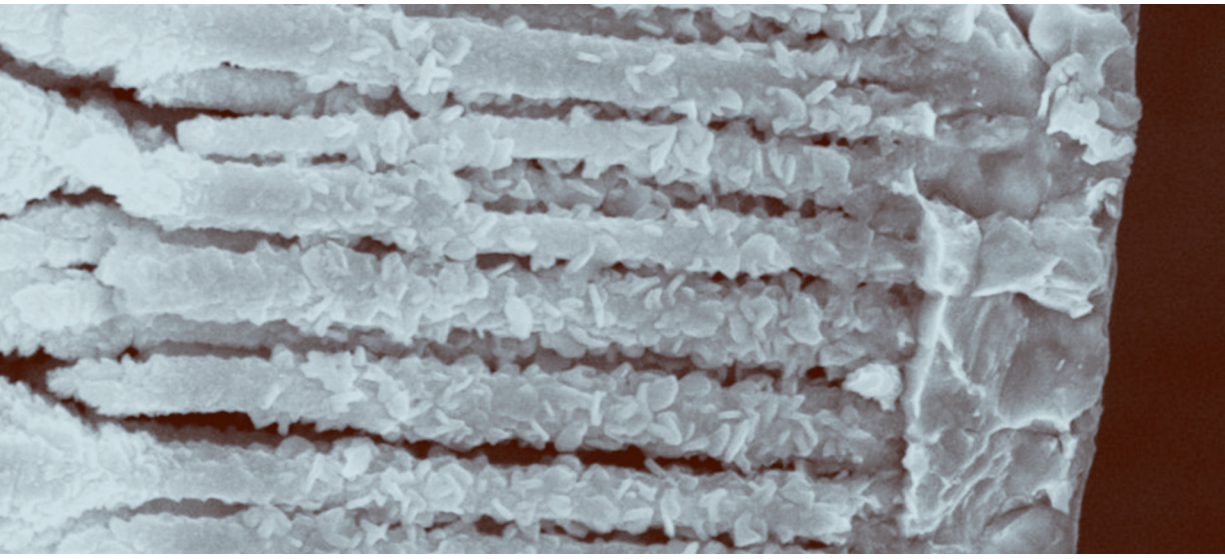
Vetenskapsrådet

INTERNATIONAL EVALUATION OF INORGANIC CHEMISTRY, 2008



VETENSKAPSRÅDETS RAPPORTSERIE 15:2008

INTERNATIONAL EVALUATION OF INORGANIC CHEMISTRY, 2008

International Evaluation of Inorganic Chemistry, 2008
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VETENSKAPSRÅDET
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Cover Photo: The picture is from Kristina Edström, Uppsala University, and her research. It shows antimony nano-particles electrodeposited on to copper nano-rods to be used as an anode for a 3D Li-ion micro-battery.
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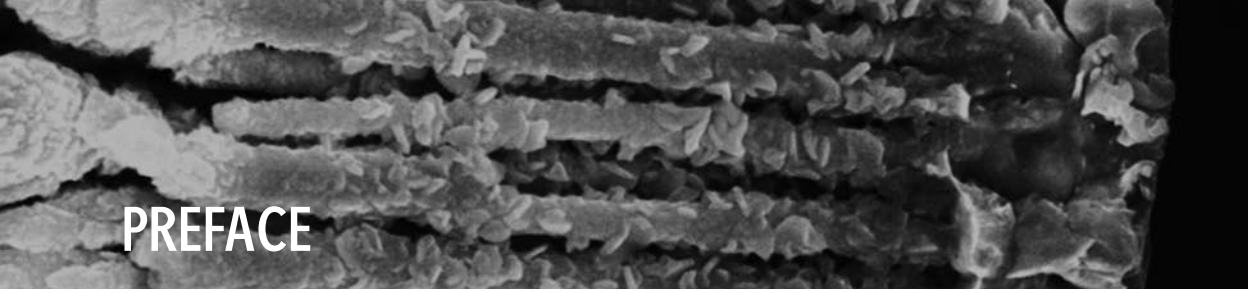


PREFACE

The Scientific Council for Natural and Engineering Sciences supports after national priority the qualitatively best research and the best researchers in Sweden. The Scientific Council awards grants for research projects totalling approximately SEK 970 million annually for Swedish basic research within natural and engineering sciences and mathematics. The essence of the task is to support basic research projects which can maintain Sweden's position at the forefront of research. Funding is given to the best researchers and their research projects, irrespective of their location in the country.

A great responsibility for the Scientific Council is to provide for the breadth of the Swedish basic research and the Scientific Council is working continuously with the renewal of the research, international co-operation and equality.

Another responsibility for the Scientific Council is to evaluate the research and the researchers funded by the Scientific Council. These evaluations serve as an independent verification on how the Scientific Council has succeeded in funding of the evaluated research area. The evaluations constitute an important instrument for strategic priorities. The Scientific Council regularly engages experts, national and international, for different assignments e.g. for evaluations of the research funded by the Scientific Council.

This evaluation report is an international evaluation of Inorganic Chemistry in Sweden.

December 2008

Arne Johansson

Secretary General
Natural and Engineering Sciences

To the Swedish Research Council

A panel of international experts was appointed in February, 2008 by the Scientific Council for Natural and Engineering Sciences, given the task of carrying out the evaluation of Inorganic Chemistry. The evaluation took place during 30 March – 5 April, 2008. During these days the grant holders under review presented their research activities to the expert panel. The panel also interviewed the grant holders during that time.

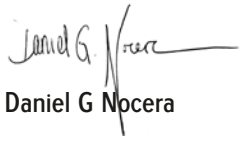
The present document reports the findings and recommendations of the expert panel, which considers its task fulfilled. According to the terms of reference of the expert panel, the international members take full responsibility for the report.

5 April 2008

Kim R Dunbar

Helmer Fjellvåg

Erik Larsen



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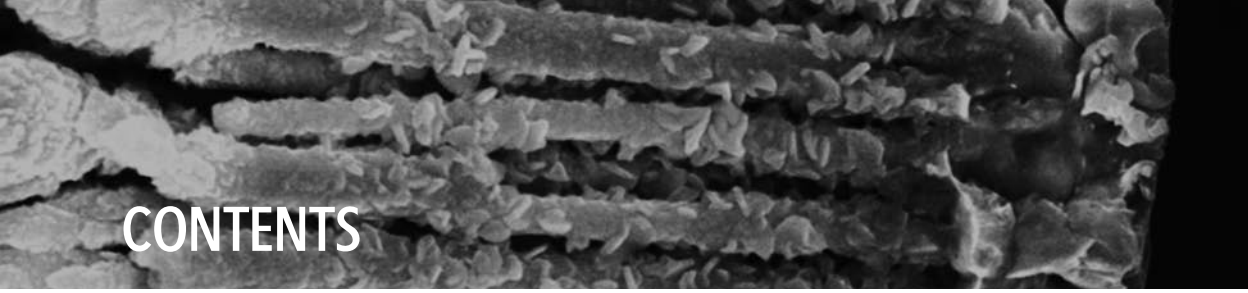

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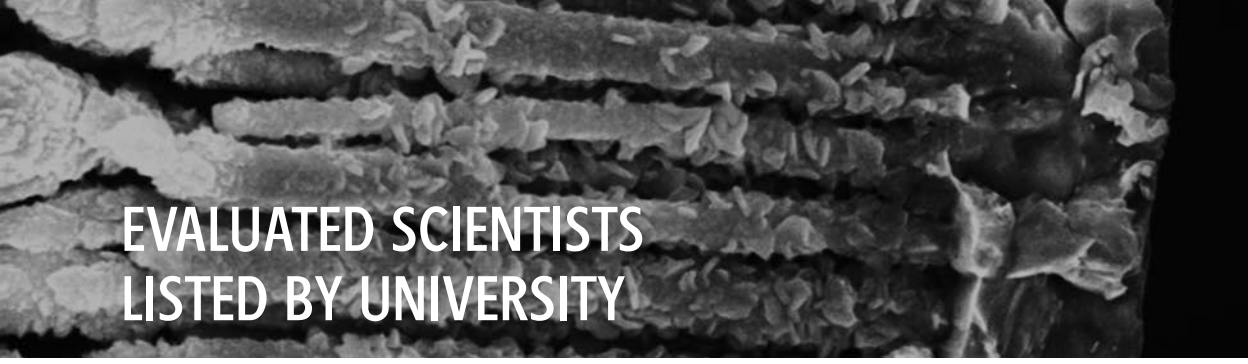

EVALUATED SCIENTISTS LISTED BY UNIVERSITY

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Umeå University

Per Persson
Staffan Sjöberg

Uppsala University

Mats Boman
Yvonne Brandt Andersson
Jan-Otto Carlsson
Kristina Edström
Ulf Jansson
Gunnar Westin

GENERAL PART OF PANEL REPORT

Contents

1. Scope of the review

The main part of the report consists of an expert panel's reviews. Twenty-nine scientists and their research supported by the Swedish Research Council (at eight universities) in the field of Inorganic Chemistry are reviewed. Each review in this report includes an evaluation of the research and recommendations based on the work accomplished over the past five years (2003–07) and the proposed future research.

The expert panel also expresses its international viewpoints on the status of Inorganic Chemistry research in Sweden, the strengths of the research topic and how to enhance its level and internal coherence. In addition, the panel advises on the balance of research supported by the Swedish Research Council within the various subdisciplines of Inorganic Chemistry. Finally, the panel makes some additional recommendations on research funding to scientists in Sweden, and gives advice on the balance among the various fields of Chemistry.

Strong support for the field of Inorganic Chemistry is crucial for the advancement of other research fields, such as Nanotechnology, Biotechnology, Environmental Chemistry and Materials Science. In particular, Inorganic Chemistry is poised to become a major player in solving the impending energy challenge confronting us this century. To this end, if Sweden is to contribute to the global efforts already launched to address the energy challenge, as well as to the advancement of other fields, key measures must be taken to ensure the vitality of Inorganic Chemistry and its prominent role in science in Sweden.

2. Inorganic Chemistry in Sweden: general observations

Research in the field of Inorganic Chemistry spans many topics. At its heart is a fundamental understanding of structure and bonding in molecules and materials, and use of this knowledge in potential applications. The concepts of Inorganic Chemistry are typically formulated in the context of design, synthesis and relationships between structures and properties, and theoretical analysis (make, measure, model). The make–measure–model approach to developing the chemistry of metals leads to the discovery of new compounds and materials that play key roles in areas as diverse as catalysts, components of renewable energy technology, clean and efficient process technology, sensors, drugs, implants, consumer electronics, information and communication technology (ICT) and nanotechnology.

Inorganic Chemistry research in Sweden funded by the Swedish Research Council is solid, and excellent in several subtopics, but clearly lags behind leading efforts worldwide. In most groups, the principal investigators' (PIs) productivity is good to excellent, but relatively few articles are published in leading journals and the work is not, in general, heavily cited. The combination of these two indicators led the panel to conclude that some PIs are failing to tackle problems at the frontline of their areas of focus.

Sweden spends an admirably large portion of its GDP on science and technology. While the share of public funding is fairly comparable to those of many other OECD countries, its industrial R&D component is unusually large. This situation implies that basic research is not particularly well funded in Sweden. Establishing priorities at national level and/or by the Research Council is recommended. This should ensure that such fields as Inorganic Chemistry, which represent the underpinning of future technologies, receive funding support that is internationally competitive.

The activities of the Swedish Research Council's Scientific Council for Natural and Engineering Sciences reflect the importance of this field. The Scientific Council supports several excellent Inorganic Chemistry projects, but not all Research Council projects with aspects of Inorganic Chemistry are covered in the present review and report. A few of those reviewed could well have been assigned under other headings, such as Physical Chemistry, Inorganic Biochemistry and Materials Science.

The panel has noted that recent reorganisations at many universities have resulted in the disappearance of Inorganic Chemistry departments. Chairs in Inorganic Chemistry seem to be rarely advertised or filled. These developments have caused considerable frustration amongst both senior and junior staff, and are contributing to general uncertainty about the fate of Inorganic Chemistry in Sweden. The undermining of Inorganic Chemistry in Sweden is in strong contrast to the international trend. It is recognised that com-

petence in Inorganic Chemistry is essential if many other, diverse priority fields in our society are to flourish.

Whether the profile of Inorganic Chemistry in Sweden is optimal is questionable. No unambiguous answer can be given since the panel has not been provided with a comprehensive overview of Inorganic Chemistry efforts in Sweden and collaboration with related fields. The panel has, however, noted that very few activities are under way in the fields of Coordination Chemistry, Bioinorganic and Organometallic Chemistry. The few groups involved in such endeavours are carrying out work that is very good to excellent. Nevertheless, the panel notes that, on the whole, the field of Inorganic Chemistry in areas other than Materials Science and Nanoscience needs to be strengthened.

The panel noted that most recipients of Research Council grants are, understandably, very concerned about how to fund their own salaries for research. It is fairly typical for them to use part of their Research Council grant for their own salaries. The panel was surprised to note the low level of university funding for young researchers, lecturers, associate professors and professors. Based on their knowledge of international programmes, the panel members expected the universities to cover at least 50% of salary, for the grant recipients' teaching and administrative duties, but this is clearly not the case. If the panel's observation is correct, the universities have exploited the Research Council's salary funding to expand their activities (part-time project funding). Senior staff, too, are paid from Research Council funds. Sweden's current university strategy of funding salaries from research grants for many months has burdened the system by providing additional resources in teaching, research training, and administrative tasks for overinflated faculties. This has created challenges with respect to research funding, external recruitment and establishment of new types of activity at a given institution. Obviously, university budgets are not equipped to absorb fully paid positions at all faculties. The present situation is detrimental: immediate changes are needed in the short term and a long-term solution should be sought.

Most Research Council grants are fairly small and provide minimum funding for completely free basic research. Many current grants are dimensioned for single individuals amounting to SEK 600,000. Nonetheless, Research Council funding is highly appreciated by researchers, both as confirmation of the quality of their work and a means of securing additional funding. Clearly, the Council plays a very important role in the funding of research in Sweden. The panel sees an obvious need for a significant increase in the size of Research Council grants, and a model where colleagues could team up and compete for larger grants for basic research programmes lasting three to five years.

3. Level of research funding

Thanks to advances in ligand design, structure-analysis methods and various forms of spectroscopy, the impact of Inorganic Chemistry has grown tremendously in the last decade. As a result, investments in this discipline yield unusually large returns. To flourish, Swedish Inorganic Chemistry requires adequate funding and staff. Funds are needed for major equipment and replacements, but also, and even more importantly, to support students and researchers at all levels. Financial straits are evident at almost all institutions and have, in several cases, resulted in decisions not to fill a Chair in Inorganic Chemistry after the holder's retirement.

Inorganic chemists in Sweden can obtain support from several sources besides the Swedish Research Council, such as the Swedish Foundation for Strategic Research (SSF), the Swedish Foundation for International Cooperation in Research and Higher Education (the STINT Foundation), the Swedish Agency for Innovation Systems (VINNOVA), private foundations, industry and increasingly, the European Union. These funds strengthen applied aspects of their research or projects at interfaces with Materials Sciences, Biosciences or Nanosciences. The basic science of Swedish Inorganic Chemistry nonetheless remains underfunded. For this reason, the Swedish Research Council is commended for maintaining the unrestricted nature of its grants — a principle that affords optimum flexibility for researchers. However, as mentioned above, the impact of Research Council funds is lessened by the need for faculties to use them to supplement salaries. The Research Council appears to be paying special attention to the needs of younger scientists through its excellent four-year and six-year programmes. Nationwide, through its Scientific Council for Natural and Engineering Sciences, it currently funds about 135 Junior Research positions (Assistant Professors) and some 80 Senior Research positions. These initiatives should be sustained.

The panel notes that the Research Council has provided support for a number of PIs' proposals that represent fairly similar research at the same institution. The expert panel found this confusing, since it impeded the members' task of evaluating each person's individual contribution. The panel recommends that, in the future, Research Council should support only one proposal in a particular research area for a given institution. This strategy will require larger research grants, but a clear distribution of responsibilities and a strong focus on collaboration from the early planning stage of the projects will, it is believed, be of considerable advantage. In this vein, the panel also argues that Sweden is in a position to set up world-renowned groups, in such fields as Materials and Solid-State Chemistry.

Several groups indicated that they have received substantial funds for equipment and infrastructure from external sources. In this respect Inorganic Chemistry appears to have well-equipped and modern laboratories. However, there are several examples of situations where researchers do not have adequate access to the requisite characterisation tools owing to lack of funds for service support, or lack of dedicated technical staff. These matters should be addressed at the university level.

The panel was distressed to find that excessive and increasing teaching workloads are substantially reducing the time PIs can spend on research. However, the panel lacks sufficient information on the entire workload situation and a perspective on staff recruitment needs and the terms on which the recruits would accept positions. Nevertheless, it is unacceptable that the universities do not guarantee at least 50% of staff's time (and salary) for research. These matters should be settled before new positions are filled.

Research Council grants cannot be used for funding postdoctoral researchers in Sweden by providing tax-free fellowships, only for normal appointments. The panel stresses that postdocs are essential for the realisation of major contributions to high-risk projects. If the limited appointments of postdocs are a result of most PIs' need to fund themselves through Research Council grants it is understandable, but most unfortunate. The entire issue of funding and the number of staff and postdocs needs to be carefully evaluated by the Research Council and other authorities. The panel also note that some researchers suffer from isolation from the international scientific community, perhaps owing to their lack of earmarked travel funds. A modest amount of seed money for travelling and establishing international collaboration would go a long way towards remedying this problem.

Despite the creative contributions of its small number of high-quality researchers in Inorganic Chemistry, Sweden does not currently play a leading role in Inorganic Chemistry worldwide. This is due, in part, to the underemphasis on Inorganic Chemistry compared with other sciences and subdisciplines in this country. The panel believes that this oversight needs to be rectified for the wellbeing of future generations in Swedish society. As pointed out above, Inorganic Chemistry is a prominent field in terms of contributing to the chemical skills that Sweden will require in the future if it is to achieve major advances in various technologies (such as materials, catalysis, corrosion and energy) that are important to society and industry. Measures to establish a strong and vital internationally organised Inorganic Chemistry community that interacts closely with other areas of science and technology should therefore be strongly encouraged. The expert panel is convinced that Swedish Inorganic Chemistry requires enhanced support and restructuring. It needs a more balanced research portfolio, retention of Senior Chairs and a rise in the number of young researchers.

4. Specific needs and future directions of Inorganic Chemistry

In the last few years, tremendous opportunities for Inorganic Chemistry worldwide have emerged. New investments in this field are imperative, especially given its decline in terms of Swedish research over the past decade.

An initial issue concerns the balance between Inorganic Chemistry and other fields of Chemistry. The unfortunate trend of departments being organised with no regard for the detrimental effect on the visibility of Inorganic Chemistry is exacerbating the weakening of this field. This trend has also bred considerable pessimism, judging from the comments of numerous researchers evaluated. Some believe that Inorganic Chemistry, as a discipline, is set to disappear from the landscape of Swedish research. The facts support this notion: Divisions of Inorganic Chemistry have become rare and professorships are increasingly not being replaced. Some leading universities (such as Lund) have relegated the teaching of Inorganic Chemistry to staff members from three different departments.

To allay some of this pessimism, an *esprit de corps* should be developed among the Inorganic Chemistry community by organising convenient meeting places and developing common strategies for teaching and research. At local university level, an Inorganic Chemistry faculty should not be split among other subdivisions of Chemistry, or between Science and Engineering. Certain decisions that have led to such fragmentation should probably even be reversed. The panel stresses that Inorganic Chemistry in Sweden is in danger of losing its international profile, unless prompt nationwide action is taken to unify the discipline.

A second issue deals with the balance between Inorganic Chemistry and more technology-oriented fields such as Materials Chemistry and Science, Biochemistry and Biotechnology, Nanochemistry and Nanotechnology. For these areas to fully benefit from Inorganic Chemistry, a flourishing Inorganic Chemistry community needs to be established at more institutions by supporting a critical mass of faculty members with international recognition of the quality and novelty of their research.

A third issue deals with the balance between Solution Chemistry (including Coordination, Bioinorganic and Materials precursors), and Solid-State Chemistry (including materials, corrosion and electron microscopy). This balance must be reconsidered in view of broader strategies connected with technological fields and applications. New directions in Inorganic Chemistry emerge continuously, some driven by advances in experimental science and others by conceptual breakthroughs. It is important for the Swedish Research Council to be open to new opportunities and willing to support them as early as possible.

A fourth issue is the Inorganic Chemistry profile of different universities. To some extent, they have already developed divergent profiles according to local requirements. Uppsala University's profile, for example, is directed towards Materials Chemistry owing to the excellent scope for research afforded by the Ångström Laboratory and interactions with Physics groups. At Umeå University, activities in Solution Chemistry dovetail with activities in Biochemistry and Geochemistry. The panel recommends giving further attention to the issue of increased specialisation among the universities.

A fifth issue deals with the number of PIs (or individual research groups) within the same area of Inorganic Chemistry at a given institution. There is obviously a need for a clear leadership, i.e. a Chair. Existing Chairs should take responsibility for developing and promoting Inorganic Chemistry in Sweden and improving the coherence among scientists in the Inorganic Chemistry community. One clear recommendation is to convene all Inorganic Chemists (faculty and group leaders) for two or three days in an isolated location to devise a national plan for developing the field in the decade ahead. The assembled group should propose a proactive plan for future areas, such as energy and nanomaterials — topics in which Inorganic Chemistry is certain to contribute to major advances. The profile of Inorganic Chemistry can also be enhanced by achieving synergy between scientists with common interests who team up in order to exert a greater impact. This must not, however, conflict with the PIs' individual responsibility and freedom.

To maintain balance among existing research efforts and allow growth in important new directions, careful thought should be given to restoring, or even augmenting the number of fully funded laboratories in Inorganic Chemistry in Sweden. Although, on the whole, the various areas of Inorganic Chemistry are fairly well balanced, it would be wise to boost efforts in Coordination and Bioinorganic Chemistry and in aspects of Inorganic Chemistry that are fundamental to Materials Science and energy research.

There is an urgent and continuous need for sufficient financial support to employ graduate students. The expert panel notes that for most investigators such support has by far the highest priority. A reasonable number of graduate students is essential for a thriving research effort in Inorganic Chemistry, in the broad sense, and is essential if the PIs are to be internationally competitive. In the short term, paramount recommendations are for requests for student support to be granted whenever possible and for strategies for national training (advanced Inorganic Chemistry courses) of PhD students to be developed. The expert panel has not noted significant efforts to form collaborative research programmes. This activity is highly recommended and should be encouraged by the Research Council in the short term.

Finally, the neglect of Inorganic Chemistry in Sweden is ill-advised and out of step with the rest of the world. Some departments around the world that have unwisely eliminated Inorganic Chemistry from their research curriculum in recent years are now scrambling to fill positions in Inorganic Chemistry. This renewed realisation of the need for a healthy Inorganic Chemistry programme is tied to one important emerging global driver. The greatest challenge facing our global future is energy, and the solution of the energy crisis is the key scientific problem we face in the 21st century. Of the sciences that will help to solve energy problems, Chemistry and especially Inorganic Chemistry are fundamental. Developing cheap photovoltaic materials will require the design of new metal-based semiconducting materials. From the storage viewpoint, new battery and capacitor materials will be needed. New electrolytes must be discovered that transfer metal ions quickly, and new metal-based electrodes (and architectures) are needed for high-energy density. If storage is to be achieved through fuel production, new catalysts are needed that can effect small molecule transformations with a bearing on energy. This is the essence of Inorganic Chemistry. By neglecting Inorganic Chemistry, Sweden will largely exclude itself from participating in one of the most important endeavours of this century. In contrast, most of the scientific world views Inorganic Chemistry as one of the leading areas of science for the 21st century — outdistancing Biology, Materials Science and other disciplines owing to its central role in solving our energy problems. It is an imperative for the Swedish Inorganic Chemistry community to embrace this new world view of Inorganic Chemistry and move their science forward, proactively addressing and applying their expertise to these emerging areas relating to energy problems.

This urgent need for Inorganic Chemistry to play a central role in energy issues, Biochemistry and Materials Science must be addressed by the projects in this review. It becomes the responsibility of the institutions, the Swedish Research Council and the scientists it supports to lead the way by taking advantage of the freedom afforded by the Council to convey the excitement and importance of Inorganic Chemistry in Sweden by working at the forefront of the key problems in science today.

5. General structural issues in Chemistry

A lack of funding for faculties and for technical support seriously limits PIs' ability to develop and even maintain their research programmes. Owing to restricted Research Council support, many programmes have been forced to rely on large-scale funding from industry, or from agencies with defined research targets and deliverables. Short-term funding for targeted problems,

with its oscillatory nature, can be devastating to the development of top-ranked research projects of high visibility, which is an indisputable goal of the Swedish Research Council. Various mechanisms should be adopted by the Research Council to tackle the challenges presented by the vagaries of short-term extramural support. For example, more support for technical support staff is needed. Modern research requires smoothly functioning, sophisticated instruments, both commercial and custom-built. Research efficiency is significantly reduced if responsibility for constructing and operating such instruments is placed solely in the hands of the PI and graduate students. More professional technical staff are clearly required. Such measures would appreciably enhance the effectiveness of research projects funded by the Research Council.

The demarcation of Inorganic Chemistry from related fields is unclear in the Research Council. The panel has obtained no clear and complete picture on its component areas and their interface with materials research. Part of the reason for the panel's inability to assess all the issues is that it was asked to judge only those projects in the field that had received a Research Council grant during 2003–07. Thus, other inorganic chemists without a grant from the Council were excluded, although they might be receiving substantial grants from other funding bodies.

As mentioned above, too many small project groups are represented in this community. Joining forces, to form clusters of two or three PIs for a major grant application, is therefore recommended whenever appropriate. The Research Council should seriously consider the option of combined, more substantial grants (fewer if necessary) over five years (funding two to four postdoctoral researchers or PhD students) and for two or three PIs together, as proposed above.

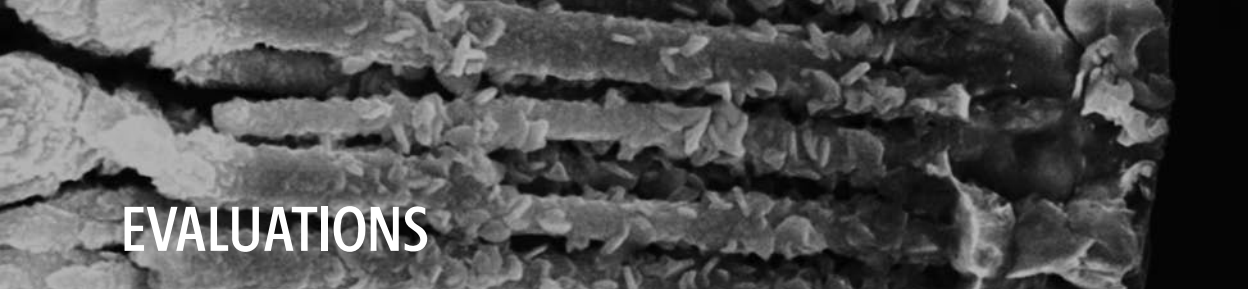
6. Other general recommendations for the Swedish Research Council and universities

A few additional comments and suggestions excluded or only touched on above are made below.

1. Promoting every eligible person to the rank of professor is unwise without the assurance of a full salary from the university covering, for example, 50% teaching and/or administration and 50% research. In principle, the salaries of permanent staff should be the university's responsibility. The panel recognises the distinctiveness of Sweden's funding scheme but urges the Research Council, along with the universities and other authorities, to review and remedy the drawbacks of the present situation. It is

hard to believe that employing financially insecure university teachers can be advantageous. The panel realises that part of this problem may have arisen from the Research Council's Junior and Senior Research Grants mentioned above (in section 3), which are, as such, highly appreciated.

2. The Research Council and the universities should send their senior and PhD students to attend important international meetings.
3. Graduate teaching is important worldwide. The Swedish community should seriously consider offering more such courses at regional, national or perhaps even international level.
4. Some Research Council project grants appear to have been renewed without the requirement of a major new research focus in the proposal. The panel recommends that all Research Council project grants should be awarded for a fixed period, and that renewal of a project grant should require a new focus of interest, whether on a related or an unrelated topic.
5. The panel notes that in several Inorganic Chemistry groups, major equipment items need replacing fairly often. It recommends that a special committee of the Research Council — which appears to exist — should scrutinise these needs on a regular basis.



EVALUATIONS

Mats Boman

Department of Materials Chemistry, Uppsala University

Synthesis of size-selected nanoparticles using LCVD and nanostructured biodevices from nanoporous alumina

Summary of the research programme

Mats Boman has been involved in two projects funded by the Swedish Research Council. In the first, nanoporous alumina was used as an active membrane in the construction of two devices — the nanobioreactor and the nanopump — and as a nanosized membrane for chromatography.

The nanoreactor uses the alumina membrane as a support for immobilised enzymes attached to the pore walls. Vertical stacking of membranes forms a multistep chemical bioreactor. Each membrane is 1–100 μm thick and the reactor can therefore be extremely compact. Nanochromatography makes use of the scope for tailoring pore size and length, as well as making pores identical, to achieve enhanced chromatographic resolution. The outcome is a set of inorganic biodevices that can work together in a multitude of ways.

A nanobioreactor needs nanopump osmosis. Putting them together creates a new device. Combining the chromatography with the nanopump enables an ultracompact separation unit to be fabricated. Combining all three devices to make a fully working bioreactor with pump and separation stages is also feasible.

Boman's intention in this work is to carry out the necessary basic research to determine the appropriate material combinations and chemistry, thereby paving the way for fully functional devices.

The second project addressed four main challenges in Nanotechnology:

1. Making sufficiently small nanosized (zero-dimensional and one-dimensional) building blocks.
2. Synthesising building blocks with a narrow size distribution and no agglomeration.
3. Assembling the nanosized building blocks into useful two- and three-dimensional structures.

4. Measuring size-dependent properties and quantifying them to tailor specific properties, the goal being to deliver new materials with unique designer properties by choosing the appropriate building-block size.

Past performance

Methodology

Boman has used intriguing methods to synthesise new nanomaterials, and his interesting and important publications of the past few years illustrate the success of this work. New methods, such as using microcoil heaters for microthrusters, are also under development. His use of microdroplets in synthesis of new nanoparticles has also attracted attention, and synthesis of Prussian Blue analogue is a genuine innovation.

Position in the area

Boman's work is of high quality and innovative. He is respected by his colleagues in the field and in the Ångström Laboratory. His research group is of acceptable size and the quality of his work was recognised in 2004 when he was promoted to a personal chair.

The number of articles published by Boman in the area is sufficient. However, with the possible exception of a 2005 publication on Prussian Blue nanoparticles, the number of highly cited publications since 2000 is somewhat limited.

Particular achievements

Use of nanoporous alumina as a template for the synthesis of new nanostructured materials in, for example, fabrication of high-aspect-ratio Prussian Blue nanotubes is highly appealing and may have many other applications.

Boman has not taken the opportunity to mark his most important publications in the output list. Nevertheless, some are discernible to the expert panel. These include the 2005 article in *Nano Letters* and the 2003 article entitled: 'Copper nanoparticles deposited inside the pores of anodized aluminium oxide using atomic layer deposition' in *Materials Science & Engineering*.

Boman's research on pore wall deposition and, in particular, sequential electrodeless deposition of palladium nanoparticles on the pore walls of anodic alumina is also worth mentioning. The impact and value of this work may increase even further as the method of alumina droplets with sequential deposition is extended to other systems.

Future prospects

Project plans

The plans presented by Boman in the oral presentation were convincing and illustrate his broad range. Several collaborative projects with colleagues from the same laboratory are planned. Teaming up with colleagues to submit joint proposals is an option worth considering. Boman is likely to continue to dedicate significant efforts to the methodology of nanoparticle synthesis. The sequential deposition technique inside the pores of anodic alumina is indeed powerful and deserves serious further investigation and funding from the Swedish Research Council.

Balance between resources and goal

Boman's current research is well funded, with good contributions from PhD students and postdoctoral associates. Boman has established several (international) collaborations with a major bearing on the project and its continuity. In the Ångström Laboratory, several advanced methods and techniques are available that will help to achieve the research goals. There is a clearly evident spinoff potential for applications in Nanomaterials Science.

Comments on the area

Position in Inorganic Chemistry

The chemistry of the formation of nanoparticles of controlled size and with tailored properties will remain important in the field of Materials Science, and Boman and his colleagues can make valuable contributions to this activity. Inorganic molecular understanding of this work is also important and interesting, and Boman and his team could perhaps pay more attention to this aspect in their future work.

Importance of the area

This area is significant from both a fundamental and a practical point of view. The area of controlled growth of nanosized particles using alumina methods is important for many possible applications.

Future potential of the area

The area of nanoparticles with tailored properties is likely to remain highly important in the next decade. Use of the alumina template permits a multitude of other applications, such as immobilising enzymes on the pore walls — a small bioreactor — to be devised. Potential applications as a sensor or for drug delivery also appear to be within reach. The potential use of functionalised

iron nanoparticles prepared in this way, in new contrast agents for use in MRI, is another apparent challenge. Boman and his team are qualified to continue to make major contributions to the area.

Overall assessment

Boman has developed a new and comprehensive approach to synthesising tailored nanoparticles by means of amorphous aluminium oxide. The spinoff of this work in terms of potential applications, as deduced from the number of patent applications, is impressive. The research funded by the Swedish Research Council has no doubt contributed to development in this area. The work is rated *very good* and further funding is *strongly recommended*.

Yvonne Brandt Andersson

Department of Materials Chemistry, Uppsala University

Light metal hydrides and magnetically ordered materials: synthesis and characterisation

Summary of the research programme

Two projects, both involving the synthesis of binary or complex metal compounds, are under investigation. In the first, Mg-metal (Mg-Y, Mg-Ga, Mg-Y-Ga, Mg-Y-Zn) and some Nb-metal alloys are being investigated as potential hydrogen storage materials. A method of growing nanosized magnesium hydride 'whiskers' under Mg-alloy hydrogenation conditions has been devised. Dehydrogenation of the hydrides leads to the interesting observation of thin-walled Mg tubes. The growth mechanism of these tubes is being explored, with the aim of correlating the structure of the whiskers and tubes with the nature of the alloying element. In the second project, the magnetic properties of mixed-metal phosphides, oxides and silicides are under investigation. The work on this project is the synthetic arm of a collaborative project involving Experimental and Theoretical Physics (P. Nordblad and O. Eriksson). The goal of the project is to acquire an understanding of the magnetic properties of complex metal silicides and phosphides, with the emphasis on defining properties of magnetic spin frustration. New manganese compounds of Mn-Ir-Si and Mn-Pd-Si compositions have been synthesised and the crystal and magnetic structures have been ascertained. The systems show the interesting behaviour of magnetic frustration.

Past performance

Methodology

Traditional high-temperature methods are used to synthesise materials in this research. Induction-heated tantalum tubes appear to be especially effective for the preparation of new magnesium alloys. The drop-synthesis method is commonly used to synthesise compounds between high-melting metals and volatile elements (such as Fe with P and Mn). Hydrogenation reactions are investigated using standard high-vacuum techniques.

Yvonne Brandt Andersson has assembled an extensive equipment base for the proposed research. Extensive instrumentation is available for structural and magnetic characterisation of new materials (such as XRD, SQUID

magnetometry, neutron scattering, AFM, MFM, XMCD and an analytical user facility with SEM/TEM/FIB/XPS). A theory modelling component is available through collaboration with Condensed Matter Physics.

The Ångström Laboratory has been invaluable to Brandt Andersson's research projects, by housing much of the above instrumentation and providing a meeting-place for chemists, materials scientists and physicists.

Position in the area

Brandt Andersson's primary interest is the synthesis and structural characterisation of intermetallic materials. Here, she is highly accomplished and has a solid footing.

Brandt Andersson confronts formidable competition worldwide in the area of materials design for hydrogen storage. Most researchers have moved on from simple hydrides, but she has an intriguing observation of suppressed temperatures for hydrogen release from magnesium hydride prepared from alloys. Nevertheless, if Brandt Andersson is to be competitive in this field, she will need to focus profoundly on the problem.

The importance of the materials originating from research on magnetism is modest to good. More generally, the work would benefit from a hypothesis-driven approach in which the synergy between measurement and synthesis would provide a roadmap for the design of new spin-frustrated materials.

Particular achievements

Magnesium hydride stores hydrogen at 7% by weight but does not release it at sufficiently low temperatures. This project pursues a strategy of lowering the temperature of hydrogen release from magnesium hydride by destabilising the hydride. This is done by alloying the magnesium with another element, such as yttrium or gallium. Brandt Andersson finds that the alloys 'decompose' on hydrogenation to produce magnesium hydride with a 'whisker' morphology. Hydrogen desorption from these whiskers is reduced by some 70% compared with nanoparticles or bulk solid magnesium hydride.

New intermetallic compounds of Mn-Ir-Si(Ge) and Pd-Mn-Si(Ge) have been synthesised and characterised structurally and magnetically. These antiferromagnetic systems exhibit suppressed ordering owing to frustration of the antiferromagnetic spins, as determined from elastic neutron-scattering experiments.

Future prospects

Project plans

The synthesis work in the research is well executed, although the expert panel obtained no clear perception of the logical path followed for synthetic targets. Such a path would appear to be essential to the planning of future projects.

In choosing future developments of the hydrogen-storage project, the panel thought it essential to define the reason for the lowered temperatures for hydrogen release from the magnesium hydride.

In the hydrogen-storage problem, Brandt Andersson appears to have chosen a fairly conservative approach to future directions. Complex hydride systems based on lithium amide have been developed in which the temperature for hydrogen release has been lowered to 285°C with the incorporation of magnesium. Given Brandt Andersson's expertise and current interest in magnesium hydride, one might expect her to tackle this kind of problem vigorously. Other materials undoubtedly await discovery.

Magnetism studies would be advanced with the design of solids exhibiting greater spin frustration. Again, this is a problem for synthesis and therefore plays to the strengths of Brandt Andersson.

Balance between resources and goal

The support provided by the Swedish Research Council sustains only a limited manpower input. The research is highly sophisticated in technical terms, involving a wide range of instrumentation and methods. The projects would benefit tremendously from additional funds for a senior position. The senior scientist would provide continuity in the research and be invaluable for the training and education of PhD students.

Comments on the area

Position in Inorganic Chemistry

Many renewable-energy schemes, especially those based on solar power, are based on hydrogen as a fuel. In this context, the research reported here has an important role to play in the design of the storage component of renewable-energy systems. Sweden currently enjoys a central position in solar hydrogen production, with a lead in the multinational Solar H2 programme. It was gratifying to hear that Brandt Andersson is seeking to integrate her research in the design of new storage materials with Solar H2 initiatives in a meaningful way.

One of the greatest challenges in Condensed Matter Science is to understand the behaviour of strongly interacting electron systems. Highly correlated electron materials can display unexpected and useful ground-state properties, such as high-temperature superconductivity and colossal magnetoresistance.

Importance of the area

As succinctly stated by Brandt Andersson, technological development advances with the creation of new compounds of matter. The fields of hydrogen storage and spin frustration are desperately in need of such discoveries. Brandt Andersson could exert a major impact by delivering new materials for these various research areas.

Future potential of the area

In the hydrogen-storage project, Brandt Andersson's expertise could be used for the discovery of new, important materials. With the ever-increasing emphasis on renewable energy and the role of hydrogen, this area's future potential looks bright.

Arguably the most pressing current issue in the field of magnetic materials is the need to discover systems in which the quantum fluctuations are strong enough to inhibit conventional order, yielding exotic ground states such as the spin liquid (derived from S=½ spin-frustrated systems). Magnetic spin frustration is believed to help stabilise such new quantum states with 'topological order'.

Overall assessment

Despite the similarity of synthetic methods and techniques for the two different project areas, hydrogen storage and magnetic materials, these areas differ markedly in intellectual focus. If Brandt Andersson is to carry out frontline research in each area, she must tackle them both with vigour. Her excitement about the synthesis of intermetallic compounds and their magnetism was evident in the presentation. The same enthusiasm was not sensed regarding hydrogen storage.

The research is rated as *very good* and continued funding is *recommended*.

Jan-Otto Carlsson

Department of Materials Chemistry, Uppsala University

Chemical film growth from vapour: aspects of mechanisms, microstructure and properties

Summary of the research programme

The research on chemical vapour deposition (CVD) and atomic layer deposition (ALD) methods endeavours to obtain a fundamental atomic-level understanding of the nucleation and growth processes involved in this deposition. The classes of materials under investigation range from oxides to metastable nitrides with variable band gaps.

The presentation focused on two projects: production of tin oxide by ALD and a metastable Cu_3N phase by ALD and CVD methods. These processes offer the potential to use chemical recognition for selective growth on desired substrate areas and laterally resolved materials structures on the molecular level. A variety of applications are proposed for the future: novel electronic materials, novel energy-storage materials, catalysis, optics, data storage, bioseparation and sensors.

The research is driven by the realisation that, although CVD and ALD processes are ideal for fabrication of the next-generation film structures, understanding of the underlying chemical interfacial processes occurring during film growth remains conspicuously lacking. The key objectives of this research concerning chemical processing of advanced materials are:
- understanding the mechanisms of the deposition process
- learning about the interplay among reactions at the film–vapour interface
- correlating the growth mechanisms and film microstructure with properties
- developing new methods of processing metastable materials and layered materials (down to monolayer stacking)
- introducing sacrificial monolayers to tailor reaction pathways and open new venues for low-temperature processing.

Past performance

Methodology

Jan-Otto Carlsson's research involves using ALD methods for copper, copper oxide, copper nitride, nickel and nickel oxide and applying CVD to copper nitride. Various approaches are used to grow the metastable copper-nitrate

phase. Experimental data, coupled with thermodynamic and quantum mechanical models, were used to evaluate the kinetics of the reaction pathway for nitride-film formation. Comparative studies of the ALD of copper, copper oxide and nitride from copper chloride were also investigated and the effect of the use of intermediate water pulses on decomposition pathways was probed.

Position in the area

Carlsson is evidently an expert in the use of CVD/ALD applications to 'classic' materials. It is clear that he has played a major role in organising a strong solid-state group at Uppsala University and devoted a great deal of time to this area of science in Sweden. His administrative duties have taken up a great deal of his time, but he has continued to work on fundamental issues related to the area of epitaxial film growth — research with major implications for industrial applications.

Particular achievements

Carlsson's group has made extremely precise measurements of the kinetics of film growth, using CVD and ALD methods. Carlsson has acquired a profound knowledge of these techniques by using relatively simple materials. This is necessary for the type of detailed knowledge that he seeks.

One important accomplishment in the area of metastable copper-nitride film growth is the realisation that a reaction pathway via surface hydroxides and/or oxides may be favourable. It was found that no film growth occurred without water being added to the growth process. Both calculations and theory point to the involvement of -OH and/or -NH_x groups.

ALD and CVD studies of tin oxide led to films from tin(IV) iodide that were of uniform thickness, as well as nearly atomically flat surfaces and very low-defect densities.

One of the most exciting discoveries is the use of ALD to fill the pores of nanoporous alumina with niobium oxide in a layer-by-layer fashion. The nanoporous alumina was later removed by means of a wet chemical technique to obtain freestanding nanotubes of niobium oxide. This is exactly the kind of application for which the ALD technique is ideal. A huge number of fundamental and commercially important topics can be pursued with this technique.

Future prospects

Project plans

The field of film growth by CVD methods is highly mature, but Carlsson appears to have carved out a niche for himself in atomic-level understanding of the kinetics and thermodynamics of film growth. In particular, he is making new contributions to the area of ALD. Carlsson has informed the panel that he is retiring in two years' time, so the future of this research will be in the hands of others, but he will certainly be able to guide and focus the efforts.

The written report refers to the future of this research in a positive, forward-looking manner. It indicates that the research is headed towards the application of these techniques to production of nanoscale aggregates and structures of precise size and properties. In addition, it notes that the use of template techniques is a rapidly expanding field but that forming multilayers and superlattices composed of alternating layers of various thicknesses, including monolayers, of 'incompatible' materials requires the design of new synthetic routes. This group is said now to be at the stage of being able to fine-tune interfacial chemistry. They need to capitalise on the knowledge they have gained.

Balance between resources and goal

If future goals include moving into new areas, particularly more applications, the resources may not be sufficient. To date, the resources appear to have been adequate.

Comments on the area

Position in Inorganic Chemistry

CVD Chemistry is a well-investigated area but may be said still to be important, although its relevance is now more on the Physical Chemistry side, with Interfacial Surface Chemistry in focus. The future impact of this kind of research is unlikely to be heavy, but will be mainly on the application side, engineering issues being paramount.

Carlsson has been a major player in the Inorganic Materials efforts at Uppsala University by a group with advanced expertise in many areas of Materials Synthesis (film and template synthesis by CVD, ALD, Electrochemistry, sol-gel synthesis and Solid State Chemistry) and numerous advanced characterisation techniques. It has been suggested by Carlsson that this part of the University would be a natural environment for a national centre for materials synthesis in Sweden.

Importance of the area

Continuing to make oxides and nitrides in thin films, thus giving an impetus to CVD and ALD for thin metal film production, is highly important.

Future potential of the area

CVD and ALD techniques are now being used to construct nanostructured solids, which opens up a wide range of possibilities for many applications. In this respect, the panel would like to see Carlsson use his expertise on some new, cutting-edge areas. It emerged in the discussion with the expert panel that he is apparently looking ahead to high-throughput synthesis, and this is a direction that his group should be taking.

Overall assessment

Carlsson's efforts have led to new concepts for film growth through application of the fundamental knowledge of mechanisms that has been acquired. This is important, but the real value of the work will lie in how this information helps to bring about key applications, especially for nanostructured materials. The research is rated as *very good* and further funding is *recommended*.

Kristina Edström

Department of Materials Chemistry, Uppsala University

Nanostructured materials for energy storage

Summary of the research programme

The research centres on providing new materials for the next generation of batteries, with the goal of creating cheaper and safer batteries with higher energy and power densities. Battery performance is limited by the materials that compose the various elements of a battery: the electrode, electrolyte and inert additives. Moreover, recent research suggests that synthetic control of the materials architectures of these different elements (including pore size, structure and composition; particle size and composition; and electrode structure down to nanoscale dimensions) could yield significant advances in battery life, performance and safety. Edström's research touches on all aspects of materials design in batteries: (i) synthesis of new anode and cathode materials, with the goal of producing higher energy density; (ii) ion transport and insertion; (iii) the properties of electrolytes and how they relate to battery performance and safety; (iv) characterisation of the electrode–electrolyte interface; and (v) an understanding of how the nanoarchitecture of the various battery elements affects performance. In all these studies, *in situ* spectroscopic techniques are important means of characterisation.

Past performance

Methodology

This research depends on a mix of synthesis and characterisation methods. Edström has enhanced her knowledge of nanoscale synthesis, which will be critical to the future of the projected research. Methods have been developed to electrodeposit nanorods of aluminium by using ionic liquids, thus allowing 3D structures to be constructed. Other methods permit creation of copper nanorods measuring 10–400 nm. *In situ* spectroscopic methods are powerful aids to this research. A range of spectroscopic techniques are used to characterise working cells. These include *in situ* XRD, Mössbauer, Raman, PES, SEM and TEM. Edström is involved in pioneering efforts to construct *in situ* neutron diffraction cells in collaboration with scientists at ISIS, the Rutherford Appleton Laboratory and the University of St Andrews in Scotland.

Position in the area

Edström has constructed a strong project directed towards examining the fundamental Materials Science needed for the development of next-generation batteries. Her work has good visibility outside Sweden. Stabilising the solid electrolyte interface (SEI) layer in lithium batteries with various electrolytes is a notable accomplishment of the group. However, several open fundamental issues, including definitive characterisation of the composition of the SEI, remain unresolved. *In situ* techniques may be applied to provide an understanding of how the SEI changes during cell operation and cycling and how conductivity of both electrons and ions in the SEI depends on composition. Understanding interphase dependence on electrode materials, electrolyte components and additives (intra-cell and intra-electrode) and designing desirable interphases are major scientific challenges that must be met if truly innovative breakthroughs in future battery devices are to be achieved.

Edström has been highly productive, although most publications are in specialised journals. Nevertheless, her work is exerting an impact.

Particular achievements

The anode surface is paramount in SEI formation and can be affected by a range of parameters, such as surface area, surface morphology and surface chemical composition. This research has examined the SEI's effect on the thermal stability and durability of batteries for different electrolytes. One interesting finding from this project is the observation of anion incorporation into the SEI, leading to enhanced thermal stability of the cell. Use of *in situ* techniques to examine dynamic properties of the materials within an operating cell is at the cutting edge of the field and Edström is commended for tackling an experiment of such complexity. The payoff will be the potential to correlate structural properties to overall cell performance.

Edström has also shown that large-volume expansion of metals during Li-alloying can be circumvented using intermetallics. In Cu_2Sb, Li^+ insertion produces Li_2CuSb, which is structurally similar to the end product, Li_3Sb, thus leading to an overall reduction in volume expansion. One especially intriguing result is that changes to electrodeposited antimony films are minimised by the incorporation of oxide and high cycling stability is consequently achieved.

Future prospects

Project plans

Several open fundamental questions, including a definitive characterisation of SEI composition, remain to be resolved. *In situ* techniques may be applied to afford an understanding how the SEI changes during cell operation and cycling and how the conductivity of both electrons and ions in the SEI depends on composition.

Edström will continue to dedicate significant efforts to constructing 3D architectures for microbattery applications. New synthesis techniques (such as ionic liquid nanosynthesis) will enable her to construct interesting architectures for current collectors, and also other electrode systems.

Balance between resources and goal

The project is well staffed, with considerable support from graduate students and postdoctoral associates, and apparently well balanced.

Edström has established several collaborations that are important to the project. In the Ångström Laboratory, several spectroscopic techniques are under development in cooperation with physicists from Uppsala University and Chalmers University of Technology. She is also well connected in the EU through programmes such as ALISTORE and SUPERLION. Through these programmes, collaborations have been established with Professors Tarascon and Simon in France. Edström also works with scientists at Argonne National Laboratory. Considering the heavy emphasis on Spectroscopy in this research project, these collaborations are important to advancing the science of the project.

Comments on the area

Position in Inorganic Chemistry

The chemistry of an operating battery will be one of the cutting-edge areas of the discipline in the years ahead. The need to increase energy density for large-scale storage calls for a detailed understanding of structure and reactivity at the molecular level.

Importance of the area

Battery devices with substantially higher energy and power densities and faster recharge times are required for storage of large-scale renewable energy. At present, there are many gaps in our basic understanding of the processes at atomic and molecular level that govern battery operation.

Future potential of the area

The area of batteries as storage media for renewable energy sources is limitless. Edström is well placed to make a major contribution to the area.

Overall assessment

Edström has developed a comprehensive approach in attacking the battery problem with intensive efforts concerning design of the anode, cathode and electrolyte. She is a driving force in the development of *in situ* measurements of operating batteries. There remains much to discover, and she looks set to be a central player in this area.

The research is rated as *very good* to *excellent* and continued funding is *most strongly recommended*.

Sten Eriksson

Environmental Inorganic Chemistry, Division of Energy and Materials, Department of Chemical and Biological Engineering, Chalmers University of Technology

Design, synthesis, structure and properties of selected complex oxides: feedback from (neutron) diffraction methods

Summary of the research programme

The projects all fall under the umbrella of 'materials design, synthesis, structure and properties'. The projects can be treated as a single programme with a focus on design and synthesis of complex oxides showing, for example, ionic conductivity, magnetic and/or electric order. Some recent focuses have been on bismuth-based double perovskite materials, such as solid solutions of $BiFeO_3$-$PbTiO_3$ and other closely related systems. Proton-conducting systems have become another prime area of research. DFT calculations guide materials design.

Besides synthesis, another focus is on instrument upgrade and on building up strong infrastructures for X-ray and neutron diffraction work. These are applied as efficiently as possible in order to find structure-property relationships among, for example, ionic conductors or magnetic systems. Thermal-analysis facilities and state-of-the-art equipment for X-ray diffraction work have made it possible to map phase transitions and follow *in situ* chemical reactions that are extremely important as feedback and for development of new chemical reaction routes. X-ray and neutron diffraction methods have been used for detailed characterisation of atomic and magnetic structure (including disordered structure). In collaboration with other groups, Eriksson also uses light-scattering to obtain information about local structure, electronic structure and coupling between electrons and the lattice. Dielectric measurements and characterisation of magnetic properties make up another important part of his group's work.

The projects focus on design and synthesis of new materials in bulk form and on correlating structure with properties. The most promising materials will be prepared as films and eventually used for various practical applications.

Past performance

Methodology

Sten Eriksson's group make high-Tc ceramics and study the materials using structural and physical methods such as magnetism, Raman, NMR and Mössbauer spectroscopies, in order to establish relationships between synthesis,-structure and properties. Neutron work is now performed at ISIS in the UK and Eriksson serves as a Swedish bridgehead to this infrastructure.

Position in the area

Eriksson's group has contributed importantly to the field of superconducting ceramics.

Particular achievements

The atomic and magnetic structures of A_2FeWO_2 (A=Sr/Ba) have been determined by combining Rietveld refinement with Reverse Monte Carlo (RMC) techniques. The magnetic structure was solved by RMC modelling for the first time.

Future prospects

Project plans

There are plans for developing state-of-the-art cells for the neutron powder diffractometer. One type is for gas control, allowing very low oxygen pressure (10-16 bar) and temperature control of the material being studied. Another cell is being developed to enable batteries and fuel cells to be studied during operation. A third type of cell permits study of hydrogen-storage ceramics at various hydrogen pressures and temperatures. These cells will enhance opportunities for work on neutrons.

In view of forthcoming efforts, with a possible location in Lund for the ESS (European Spallation Source), this group seems to be a key player in the neutron field.

Balance between resources and goal

The close involvement of Eriksson's group in the national programme for neutron scattering and the important research it is conducting prompt an unchanged level of funding.

Comments on the area

Position in Inorganic Chemistry

Eriksson's research is in Materials Science. His scientific efforts are based on the techniques, knowledge and ideas of Inorganic Chemistry. In terms of the support provided for neutron diffraction, responsibility for supporting Swedish users by giving them ready access to beam time and creating sound infrastructure for their use is of prime importance.

Importance of the area

The importance of Materials Science can hardly be overemphasised.

Future potential of the area

For many solid-state chemists and physicists, this field of investigation will remain highly relevant.

Overall assessment

Eriksson is a very important person for the Swedish neutron community, especially now that a new European Spallation Source is under consideration. His research is rated as *very good* to *excellent*. Continued funding is *strongly recommended*.

Saeid Esmaeilzadeh

Department of Physical, Inorganic and Structural Chemistry, Stockholm University

Functional nitrides and carbides of main group elements

Summary of the research programme

The research focuses on preparing and characterising new nitride- and carbide-based glasses and ceramics. While previously reported glass phases in this chemical area are limited to nitrogen content typically lower than 20%, a new synthesis method developed and patented now enables Saeid Esmaeilzadeh to extend the synthesis of oxynitride glasses to nitrogen concentrations as high as 70%. With respect to silicate materials, these nitridosilicate glasses provide very high refractive indices, with values as high as n = 2.30. Materials in this group are, at the same time, the hardest silicate glasses ever obtained, with hardness values as high as H = 13.0 GPa. High concentration of magnetic ions, such as Pr^{3+}, Tb^{3+} and Gd^{3+}, can readily be incorporated into the nitride-based glasses. This project aims at extending fundamental knowledge of synthesis mechanisms, as well as of the relationships between composition, structure and properties of nitride-rich materials. These glasses are unique and interesting both in terms of basic science and because of their high commercial potential. Parallel to the scientific development, a number of patents have been obtained. Industrial collaboration has been intensified and the fundamental research is showing results in the form of technological implementations and new products.

Past performance

Methodology

Esmaeilzadeh has developed a novel synthetic approach to N-rich oxynitride glasses, emphasising the Si-La-O-N system to date. This approach opens up the possibility of raising the N content of the Si-La-O-N system of glasses. The mechanical and physical properties of the glasses depend heavily on the N content and this results, for example, in an extraordinarily high refractive index and exceptional hardness. Work focuses on basic studies of the synthesis process and products at the atomic and microstructural levels. The research has led to patents and a spin-off company that converts oxynitride glasses and ceramics into commercial products.

Position in the area

Esmaeilzadeh is working within the broad field of oxide-based glasses and ceramics. With his new synthetic approach he has, however, opened up a new area of N-rich glasses. In this field he holds several patents and is considered by the expert panel to be uniquely placed to expand this field in novel directions, scientifically and technologically. Esmaeilzadeh is a young researcher, with very sound achievements and the potential to make important contributions to Inorganic Chemistry.

Particular achievements

Esmaeilzadeh has developed a novel synthesis method for preparing nitrogen-rich liquid phases that yields final materials in form of glasses or crystalline ceramics. He will no doubt be identified as a pioneer in this field.

Future prospects

Project plans

Esmaeilzadeh describes his primary future interest as microstructure design of functional materials, with a focus on oxynitride glasses and crystalline ceramics and with applications in energy and biomaterials. The new field of N-rich glasses undoubtedly has a bright future with respect to fundamental and applied research. The panel recommends a focus on exploring novel opportunities and properties in selected oxynitride systems. This may involve, for example, extending the Chemistry in new directions (going beyond Si-La-O-N materials) in the quest for N-rich glasses and compounds and turning to more detailed analysis of the atomic and microstructure properties of glasses and crystalline ceramics.

Balance between resources and goal

There seems to be a good balance between the resources available and the goal of the research. The more applied aspects of the research have been, and should continue to be, conducted by the spin-off companies.

Comments on the area

Position in Inorganic Chemistry

Oxynitrides, in the form of glasses or crystalline ceramics, are important inorganic materials. Synthesis of these, as well as studies of their structure and properties, is highly relevant to Inorganic Materials Chemistry and Solid State Chemistry.

Importance of the area

Glasses and ceramics are important inorganic materials. Describing and understanding the atomic and local structure of glasses remains a highly challenging field that may afford greater understanding of the group of disordered, amorphous and glassy materials. Oxynitrides represent a category of inorganic compounds and/or phases that have not yet been fully explored.

Future potential of the area

The field of N-rich glasses is expected to develop further in the future, and manufacturing of components based on such materials will find applications in broad technological areas. Further development of synthesis routes may enhance this development.

Overall assessment

The area of N-rich glasses and ceramics has major potential for further development, with respect to more detailed understanding of materials and structures at the atomic and microstructure level; extension into related chemical systems; and more applied research. The panel strongly recommends that Esmaeilzadeh should focus his efforts on expanding the Chemistry aspects and gaining more profound knowledge of the novel category of N-rich materials, which is an excellent research topic. The panel rates the research quality *very good* and *strongly recommends* continued funding.

Andreas Fischer

Division of Inorganic Chemistry, Department of Chemistry,
Royal Institute of Technology

Novel lanthanide perhalogenates as optical materials

Summary of the research programme

The aim of the project is to investigate the lanthanide perhalogenate system in order to develop novel materials with optical properties for various applications. Periodate has been shown to coordinate to lanthanide ions, forming three-dimensional networks. Additionally, these ions have the ability to condense, depending on pH and concentration, thus forming chains whose size may be varied. This makes it possible to control the concentration of ions in the solid state, thus changing the properties of the material. So far, the lanthanide/periodate system has not been investigated thoroughly, and structural information and knowledge about which phases exist are very sparse. In this project an investigation is planned using widely varying concentrations of the species involved and employing various synthetic strategies, such as hydrothermal syntheses, to obtain crystalline samples. These will be characterised structurally, mainly using X-ray diffraction techniques, in terms of their physical properties, i.e. thermal behaviour and optical and electric properties.

Past performance

Methodology

Andreas Fischer has studied Structural Chemistry by using X-ray diffraction techniques of synthesised compounds. The compounds have fallen into two groups: transition metal perhalogenates, for which a strategy was formed, and an accidental group of smaller organic molecules and their polymorphs.

Position in the area

Fischer has made important contributions to the structural chemistry of transition metal perhalogenates. Little attention had been devoted to this research previously. The synthetic work seems fairly simplistic and the reported schemes to obtain crystals, lasting from six months to three years, do not seem particularly efficient.

Particular achievements

The fact that the uranyl ion sometimes 'chooses' to coordinate both to water only and, at other times, to water and perchlorate ions appears to be an important new piece of information for the uranyl system, since the perchlorate anion has been considered a non-coordinating one to date.

Future prospects

Project plans

One major effort will be to yield improvements in teaching techniques for Crystallography, since this is an important issue for many areas of application and it is providing the group with collaborative research.

Balance between resources and goal

The previous grant was fairly small and time-limited. Still, since Fischer has mainly been supporting other groups with X-ray expertise it is questionable whether the funding should have been provided.

Comments on the area

Position in Inorganic Chemistry

Fischer is a young, skilled and thorough crystallographer. He is in close contact with larger projects and it is recommended that he should join one of them.

Importance of the area

It seems a good idea to study periodates of heavy metal ions in order to obtain compounds with useful non-linear optical properties that depend on heavy cations and non-symmetric heavy anions, both with low optical absorption.

Future potential of the area

There will be a continuous need for X-ray structure determination in the future.

Overall assessment

Fischer appears to be a skilled crystallographer and he should be able to serve the department as such. The research is rated *good*. Continued independent funding is *not recommended*.

Julius Glaser

Division of Inorganic Chemistry, Department of Chemistry,
Royal Institute of Technology

Studies of speciation, structure and dynamics of coordination compounds

Summary of the research programme

For many years, speciation, structure and dynamics of coordination compounds in solution have been among Julius Glaser's topics of study. Molecular mechanisms for chemical reactions in solution constitute the key for understanding and control of Chemistry, including environmental, life and industrial processes. The goal of his project is to expand knowledge of these fundamental processes in Inorganic Solution Chemistry by studying the kinetics and mechanisms for formation and decomposition of molecules, ligand exchange and electron transfer reactions for metal-ion complexes. Both irreversible reactions and reactions at chemical equilibrium are studied. Except for the very slow processes, the latter information has only recently become accessible, thanks to advances in pulsed multinuclear NMR techniques.

For a full and detailed account of molecular processes in solution, a study of reaction dynamics must be preceded by an investigation of equilibria and the structure of the species involved. The approach has therefore been to use a combination of several experimental and theoretical methods to obtain as much relevant information as possible on the chemical systems studied. The main idea is that such a comprehensive approach in solving mechanistic problems will provide a new insight into the molecular scene of the exchange pathways.

A new project involving studies of production of suprapure solid silicon is proposed. It is aimed to create electron-hole pairs, using ionising radiation, and then use the free electron to reduce silicon (IV) compounds in methanolic solution to elementary silicon, which can be used in silicon solar cells and for making electronic chips.

Past performance

Methodology

The expert panel was asked to carry out a full evaluation of the research conducted during 2003–07. However, most of the work presented was outside this time frame. Glaser started this project, concerning a family of metal–

metal bonded compounds with 'naked metal-metal bonds', a long time ago. He has reached interesting and important results in the past, and over the past decade this has attracted scientists to use these results in theoretical studies, for example. Collaborators elsewhere (in Hungary), moreover, were attracted by the chosen system of Tl-Pt cyanides. The methods of characterisation are primarily X-ray Crystallography, advanced NMR, Vibrational Spectroscopy and solution studies.

Position in the area

Glaser's past work was of high quality and innovative, but in recent years little new work has emerged from the project. On the other hand, he is respected by his colleagues in the field, as illustrated by the appearance of his name as a (non-corresponding) coauthor on publications from foreign laboratories. The number of articles published by Glaser in the area is satisfactory in every year, although it has decreased since 2000.

Particular achievements

Glaser's research on Tl, Pt and cyanide, which started in the 1980s, attracted much attention. It led to many good publications, often with other authors, and showed several new and unusual structures of interest to theoretical chemists. Thermodynamic, structural and dynamic properties of the compounds in solution, as well as their light sensitivity, were studied.

Future prospects

Project plans

The plans described by Glaser in the oral presentation indicate a totally new direction devoted to production of ultrapure solid silicon using ionising radiation. After reduction by free electrons of silicon(IV) compounds in methanolic solution to Si, the latter was proposed for use in silicon solar cells and for making electronic chips. It was not clear to the panel whether Glaser is qualified to undertake such a difficult new project in an area where he has not worked before. Moreover, production of highly pure silicon from an organic solution is highly unlikely.

Balance between resources and goal

Glaser's past research was well funded, with good contributions from PhD students and collaborators. Glaser has established several (international) collaborations with a bearing on the project, but he has no proven record for the newly proposed work.

Comments on the area

Position in Inorganic Chemistry

Work on the chemistry of the Pt-Tl cyanides began in the 1980s but, in fact, ended almost entirely before the time frame of the present evaluation started (2003). The topic was a strong one, but since 2003 the position has gradually weakened and few new results have emerged.

Importance of the area

Solution Inorganic Chemistry is an important and relevant field to study, and one that should be maintained in Sweden.

Future potential of the area

Solution Inorganic Chemistry is an important area not pursued by many Swedish inorganic chemists.

The prospects for Si production is difficult to address since no plan has been drawn up and presented by Glaser.

Overall assessment

Glaser made important contributions to the fields of Molecular and Solution Coordination Chemistry between 1983 and 2003. This work was well cited and attracted several partners from abroad, resulting in joint publications and many citations from other groups. However, during the evaluation period (2003–07) not much work has been added. The research is rated *good* by the panel. The plans for a proposed new project on synthesis of ultrapure Si, on the other hand, are considered less than realistic and *not recommended* for funding.

Mikael Håkansson

Organometallic Chemistry, Department of Chemistry, Göteborg University

Absolute asymmetric synthesis

Summary of the research programme

This project concerns new labile conglomerates that may constitute the basis for:

1. A conceptually new method for enantioselective organic synthesis. If the labile conglomerate can be resolved into an enantiopure reagent or substrate complex, the chirality can subsequently be transferred to a large number of stereochemically inert organic molecules.
2. Isolation of inorganic stereoisomers. Enantiopure, labile complexes are inherently interesting, but even such a basic task as resolving complexes of five, seven or eight coordinates has remained a challenge not tackled until recently.
3. Bulk synthesis of enantiopure materials. In view of the increasing use of biomaterials, an ability to prepare new materials with 100% yield and 100% enantiomeric excess is highly attractive. Lability is not a problem when the desired product is an insoluble material, since racemisation in the solid state is then less likely.
4. Information concerning the origin of biological homochirality. Labile conglomerates may have been instrumental in the creation of optical activity on prebiotic Earth. With the growing number of spontaneous resolutions of labile conglomerates, crystallisation-induced asymmetric transformation will be an increasingly likely mechanism for the genesis of biomolecular homochirality.

Past performance

Methodology

Apart from advanced organometallic synthesis, absolute asymmetric synthesis (AAS) is the most important experimental method employed in this project. In addition, circular dichroism and single-crystal X-ray diffraction are invaluable tools.

Position in the area

Mikael Håkansson is exploring an intriguing basic issue in Chemistry, the fundamentals of chirality, by studying the chirality of a well-chosen range of relevant and interesting coordination and organometallic compounds.

Generating and purifying enantiomers, starting from achiral materials, without huge auxiliaries in an appropriate temperature window, are a remarkable and important achievement. The early publications on the AAS were in top journals and have been well received in the field.

Particular achievements

In addition to the design and synthetic work in the field of AAS, Håkansson's group has developed an important method using CD spectroscopy on solid samples. This method not only identifies the correct enantiomer, but also permits quantification of the enantiomeric excess in the powder of the labile product. Use of this method is crucial to the progress of this project, and one key goal is to expand the sample range into air-sensitive molecules. Publications have already appeared regularly in high-ranking journals.

Future prospects

Project plans

The inherent advantages of the AAS method as developed by Håkansson, compared with traditional enantioselective synthesis or resolution techniques, are significant. First, both enantiomers are available equally and, in principle, on a large scale — even up to 100% yield and enantiomeric excess. Secondly, no optically active material needs to be discarded and no catalyst or auxiliary needs to be added. Håkansson presented his plans for the future clearly and enthusiastically.

Balance between resources and goal

Håkansson's research project has been relatively small to date, with little involvement of PhD students supported by the Swedish Research Council. Håkansson has good ideas and has presented clear plans for the future. Since he has the capacity to handle a larger group, extension of the funding is strongly recommended by the expert panel. The work is performed in an Organic Chemistry department, apparently owing to the absence of a related Inorganic Chemistry group at Göteborg University. This fact should not impede the funding.

Comments on the area

Position in Inorganic Chemistry

Håkansson has discovered and developed an appealing new area of Inorganic Chemistry, studied by only a few other labs worldwide. Thanks to his recent publications, his position is well established.

Importance of the area

The area of chirality in Coordination Chemistry is of profound fundamental interest, and the outcome of research in this area will be very important outside the Inorganic Chemistry field as well. Crystallisation-induced symmetry breaking, which may eventually result in highly reactive enantiopure crystals of stereochemically labile reagents, is of major potential future importance.

Future potential of the area

The broad field of chirality in Coordination Chemistry is likely to remain a major area of research that is relevant to Organic Chemistry and Biochemistry.

Overall assessment

Håkansson has made an important and fundamentally very interesting finding in Coordination Chemistry that warrants further development and extended funding. The overall quality of his research is rated as *very good* to *excellent* by the panel, which *strongly recommends* maintaining and extending the Swedish Research Council's funding.

Ulf Jansson

Department of Materials Chemistry, Uppsala University

Synthesis and characterisation of new nanostructured carbon materials

Summary of the research programme

The main objective is to synthesise and characterise various types of complex carbide structure using magnetron sputtering as the main materials-growth technique. The project is threefold: (i) new MAX phases of three or more components (where M = Ti, V, Fe, A = Si, Al, Ge and X = C); (ii) self-structuring carbide films; and (iii) carbide-based nanocomposites. All three subprojects represent emerging classes of thin-film materials with major potential in many applications, but where fundamental studies are required to make full use of their capabilities. Within this project, experiments are combined with theoretical DFT calculations to predict and synthesise new MAX phases, nanocomposites and systems with self-structuring behaviour. Deposited films are characterised using, for example, X-ray diffraction, X-ray photoelectron spectroscopy and electron microscopy methods. Their mechanical, electrical and magnetic properties are also studied. These studies include, in particular, the relationship between process parameters and microstructure, and also relationships between microstructure and properties. One clear objective is to establish the general trends of how these structures are formed and, moreover, to benefit from these trends in predicting and synthesising future thin-film structures. Examples of materials are the MAX phases mentioned above. Another group of target materials is nanocomposites, such as nc-TiC/a-C, where controlled 'doping' with other elements (such as Al, Ni and Fe) can help in the design of, for example, low-friction and electrical-contact materials. In the past year, preliminary studies on graphene, both for a model system (carbon nanosheets) and for products based on the current synthetic process, have been carried out.

Past performance

Methodology

Ulf Jansson is working on a wide range of novel aspects of carbon-based materials, using magnetron sputtering as a major synthesis technique. He focuses on several types of emerging classes of thin-film materials: multi-component carbides and nitrides, MAX phases, self-structuring carbide

films and carbide-based nanocomposites. Development of novel carbon-based materials combines experiments and theoretical calculations, and has major innovative potential.

Position in the area

Jansson is internationally well recognised in the area of thin-film technology and carbon-based materials. A large number of high-quality publications illustrate the novelty of his research and he shows an excellent ability to collaborate and enhance science at the interface between Chemistry and Physics.

Particular achievements

Jansson's recent achievements with respect to novel carbon materials include nanocomposites made at low temperatures, which have potential uses for wear-resistant electric contacts and materials that are self-adaptive to external changes, and applications in Tribology.

Future prospects

Project plans

The field of novel carbon materials has a major potential for future basic and applied research. Interaction with computational modelling of electronic properties and stability will help in selecting and understanding materials and concepts. Jansson's plan to extend his efforts in synthesis and characterisation of new designed nanocomposites fits in excellently with this strategy. Jansson intends, moreover, to develop new synthesis routes to graphene and to include graphene in future nanocomposites. In the carbide area, one ambition is to develop design concepts for new materials for use as sensors, electrical contacts and tribological contacts. This will combine fundamental research and more applied projects. Other major topics are interfacial phenomena in nanocomposites and materials design by 'controlled' phase transformations.

Balance between resources and goal

Jansson is well placed at Uppsala University, with excellent facilities at the Ångström Laboratory for both synthesis and characterisation of carbon-based materials and nanocomposites. This also applies to his collaboration with theory and Physics, as well as with organic chemists with respect to graphene chemistry. There is close correspondence between resources and goals in future project plans. The fundamental research is likely to lead to innovations and hence to more applied projects with various types of funding.

Comments on the area

Position in Inorganic Chemistry

Carbon-based phases, nanocomposites and graphene are central inorganic materials that still possess major potential for new science and technological implications. Methods of making such materials, and the use of theory and modelling to help in making predictions on stability and properties, are central to Materials Chemistry and Science.

Importance of the area

A fundamental understanding of the structure, stability and electronic and physical properties of inorganic materials is important for future applications in many technological areas. This understanding should include a profound grasp of how properties are modified by using nanosized particles and nanocomposites. Inorganic Chemistry has important tools for synthesising and characterising carbon-based materials, in bulk and nanostructured forms.

Future potential of the area

Design of novel nanostructured materials and composites, as well as synthesis of graphene and studies of its properties, whether separately or in composites, represent emerging fields with a major potential for new science and innovations.

Overall assessment

Jansson has made a large number of very interesting advances in carbon-based materials and nanocomposites. His plans for the future show great promise of new insight in fundamental aspects of synthesis and properties of carbon-based materials, including nanocomposites. This research involves close collaboration with groups in Physics, modelling and Organic Chemistry. The expert panel rates his research as *excellent* to *outstanding*. Continued funding is *most strongly recommended*.

Lars-Gunnar Johansson

Environmental Inorganic Chemistry, Division of Energy and Materials, Department of Chemical and Biological Engineering, Chalmers University of Technology

Mechanisms of atmospheric degradation of Al, Mg and MgAl alloys: a microscopic approach

Summary of the research programme

This research addresses the mechanism of atmospheric corrosion of light metal alloys. Recent advances in instrumentation are now used to enhance the understanding on the micro- and nanoscale. The emphasis is on studies of microstructure (intermetallic phases and grain boundaries) and on localised corrosion. The work focuses on the influence of temperature, humidity and trace substances, as well as the formation of corrosion products. A cross-disciplinary approach covering Surface Chemistry, Alloy Microstructure and Corrosion, and combining micro- and macroscopic perspectives, has been adopted. Carefully controlled lab exposures are combined with *in situ* surface probes and with microstructural investigations by FIB, SEM and TEM. The studies have pioneered the use of local electrochemical measurements (SKPFM) and AFM to investigate the influence of noble inclusions in Mg and MgAl alloy corrosion. CO_2 has been found to inhibit atmospheric corrosion of Al and Mg, which explains the tendency of Al to corrode in crevices and occluded environments. Environmental degradation is a crucial factor for light metal alloys, especially Mg-based alloys, in outdoor applications.

Past performance

Methodology

The research follows four directions: (i) high-temperature corrosion; (ii) atmospheric corrosion of light metal alloys; (iii) functional oxides; and (iv) biophotovoltaic thin-film nanodevices. The main emphases are on (ii) and (iv).The corrosion studies involve characterisation at different lengths, from nanometres to centimetres. Surface characterisation tools are particularly important, for such purposes as simultaneous study of surface topography and Volta potentials.

Position in the area

Lars-Gunnar Johansson is very well recognised in the fields of high-temperature and atmospheric corrosion. Furthermore, he has made important contributions to knowledge of oxide materials with interesting physical properties, such as superconductivity and magnetism. At present, he heads a national competence centre for high-temperature corrosion.

Particular achievements

Johansson has made several important contributions to our basic understanding of corrosion. Recent achievements include the use of novel surface probes to investigate topography and Volta potential simultaneously. This emphasis on *in situ* methodology has proved particularly important in affording a more profound understanding of the intimate relationships among surface topology, corrosion product formation, chemical composition and electric potentials.

Future prospects

Project plans

Johansson describes plans for fundamental research in the following directions: high-temperature corrosion; atmospheric corrosion of light metal alloys; functional oxides; and biophotovoltaic thin-film nanodevices. These plans comprise the joint priorities of a closely collaborating team of three Professors at Chalmers University of Technology (in cooperation with Sten Ljungström and Jan-Erik Svensson). Johansson's individual contribution to the team's plans and progress is not easily identified. One key issue is to secure a critical mass to advance science in the above-mentioned areas. Plans for the biophotovoltaics seem not to have matured to the same levels as those for the other three topics.

Balance between resources and goal

Johansson collaborates closely with his colleagues at Chalmers University of Technology and describes his activities as a team effort. This is indeed required for maintaining sufficient focus and a critical mass for all the fields of interest: high-temperature and atmospheric corrosion, functional oxides and biophotovoltaics. His leadership of the applied high-temperature corrosion centre, which focuses on formation and breakdown of protective oxides, assures the group of key resources. Overall, there appears to be a good balance between resources and the goal.

Comments on the area

Position in Inorganic Chemistry

The fundamental issues of corrosion have strong components of Inorganic Chemistry. The basic approach adopted, with the objective of understanding mechanisms, is combined with applied research in which corrosion products are characterised. The activities concerning magnetic and conducting oxides are of interest in Inorganic Materials Chemistry, with a wide range of potential applications.

Importance of the area

High-temperature corrosion and atmospheric corrosion are, in practical terms, highly important processes for materials degradation. Accordingly, there is a powerful financial driver for understanding and mitigating corrosion. Fundamental insight into these areas is important.

Future potential of the area

Continuous development of (surface) characterisation methods is providing new opportunities for fundamental studies of corrosion mechanisms. At present such mechanisms are not understood to a level at which Materials Science can benefit from the knowledge in making corrosion-resistant surfaces.

Overall assessment

Johansson's research activities span various fields of Inorganic and Materials Chemistry: high-temperature corrosion, atmospheric corrosion, functional oxides and, more recently, biophotovoltaics. The research in atmospheric corrosion is of very high quality, addressing fundamental issues and using state-of-the-art methodology. The high-temperature corrosion issues are mainly oriented towards applications and industrial needs. The expert panel rates the total activity as *very good* to *excellent*. Further funding is *strongly recommended*.

Mats Johnsson

Department of Physical, Inorganic and Structural Chemistry, Stockholm University

Synthesis and characterisation of low-dimensional materials

Summary of the research programme

The aim of this research is to develop and explore a synthesis concept that affords a high probability of forming new low-dimensional compounds. A further aim is to characterise the magnetic, electric and/or optical properties of the new compounds. The synthesis strategy is to utilise p-element cations, such as Se(IV), Te(IV), Sb(III), Bi(III) and halide ions (Cl^- and Br^-). Both groups of compounds help to cut down the dimensionality of the arrangements of transition metals in crystal structures. The chemical differences between various cations are thus utilised, since transition metal cations are generally more halogenophilic than the lone-pair cations. This fact causes the transition metals to surround themselves with both oxygen and halogens as ligands, while the lone-pair elements normally coordinate oxygen in an oxohalogenide environment only.

The synthesis concept has proved powerful for finding new compounds where transition metals are isolated to planes, chains or quasi-zero dimensional arrangements. The synthesis methods are solid-state synthesis, transport reactions, solid-gas reactions and hydrothermal synthesis.

Past performance

Methodology

Traditional materials synthesis techniques such as transport, high-temperature solid-gas and hydrothermal reaction methods are used to produce low-dimensional magnetic materials. A battery of structural techniques are used to characterise the materials. Magnetic measurements and theoretical work are carried out by a strong team of Physics collaborators.

Position in the area

Mats Johnsson collaborates extensively with five groups, four German and one French, while also extending his collaboration with Professor Sven Lidin in Stockholm. A meeting funded by the European Science Foundation (ESF) was organised in 2003 in the 'Highly Frustrated Magnetism' network, and collaboration on detailed characterisation of the magnetic properties of promising compounds has been established.

Particular achievements

Johnsson has capitalised on an ingenious design element in developing 2D materials. By using the inert lone pair of bridging chalcogenides between metals, he can terminate 3D structure and enforce 2D layers. This is quite brilliant and Johnsson is to be commended for creating this design concept, which should be useful to others. His use of Cu^{2+} ions in some of these lattices to design Kagomé lattices and other low-dimensional systems is especially interesting. This is a genuine achievement, especially since the materials were synthesised using the thoughtful design concepts invented by Johnsson himself.

Future prospects

Project plans

The study of ceramic materials will be extended by syntheses concerning the theme identified. The main focus will be on affording a more profound understanding of the role of the p-element, exemplified with Te(IV).

Balance between resources and goal

The whole infrastructure and the relatively new instruments available to Johnsson are valuable and keeping them running involves relatively low cost. The numbers of PhD (five), MSc (one) and BSc (seven) students have resulted in a fine list of publications commensurate with funding to date. This warrants continuation of funding.

Comments on the area

Position in Inorganic Chemistry

The area of magnetic spin frustration is a materials-deficient field. The number of genuine spin-frustrated systems is relatively small, primarily because not enough synthetic chemists have tackled the problem. This is changing with the likes of Johnsson, who is attempting to develop a chemical rule set for the design of low-dimensional, spin-frustrated systems.

Importance of the area

Magnetic frustration is a phenomenon of highly correlated electron systems, a cutting-edge topic in Condensed Matter Physics. Of these materials, the spin liquid is perhaps the most challenging. In a spin liquid, antiferromagnetic spins on triangles (or tetrahedra) cannot attain order owing to geometric frustration. The spins are unable to freeze in an ordered state, even at the lowest temperatures — hence the characterisation 'spin liquid'.

If the spin liquid remains disordered to the lowest temperatures, quantum effects may dominate. In this field, the universal quest is for quantum spin liquid with S=½, 2D materials. It is therefore exciting to see that Johnsson has constructed such systems, using well-defined design concepts.

Future potential of the area

The area of spin frustration and highly correlated electron systems is at the frontline of Condensed Matter Science. It is gratifying to see a synthetic inorganic and/or materials chemist attempting to provide design concepts for such interesting materials.

Overall assessment

Johnsson's group is doing interesting research in Magnetism and Structural Chemistry that is rated as *very good* to *excellent*. Further funding is *strongly recommended*.

Vadim Kessler

Department of Chemistry, Swedish University of Agricultural Sciences

Molecular precursors and molecular models of nanomaterials

Summary of the research programme

The research conducted by Vadim Kessler in the Materials for Environment group at the Swedish University of Agricultural Sciences is devoted to the development of new synthetic approaches to homo- and heterometallic complexes, using alkoxides, beta-diketonates and carboxylates as precursors for nanomaterials from mild decomposition reactions. At this stage, molecules are the primary focus; but the ultimate motivation is to use new precursors in sol-gel syntheses of catalysts, functional and protective coatings, and membranes, and also in chemical vapour deposition, solution thermolysis and molecular self-assembly. The overarching theme of all the work is an interest in molecular precursors and molecular models for nanomaterials. The synthetic work of this group has advanced the knowledge base of Molecular Precursor Chemistry based on metal alkoxide units, primarily by "debunking" the myth that reactivity proceeds by means of ligand exchange without changes in the core structure. A fresh approach to the area has emerged and is certainly of high interest to the field of Sol-Gel Chemistry, CVD applications etc.

Results to date have led to the realisation of new complex alkoxide precursors that hold considerable promise for production of useful materials, particularly for bioencapsulation and drug delivery but also for ultrafiltration.

Past performance

Methodology

Soft chemistry techniques are used to prepare new network solids based on oxide, sulfide or metal alloys with controlled porosity. The materials are prepared by synthetic modifications to organic ligands on the precursor compounds, which are decomposed by hydrolysis reactions or thermolysis in the gas phase or solid state. The idea of compiling a structural database and a set of rules for metal alkoxide reactivity is a clever one. With the right molecular precursors in hand, it is hoped that the catalytic, electronic and optical properties of materials prepared from them can be manipulated. Specific targets are microporous Zr, Hf and Ti oxide coatings on the surface of silica

for ultrafiltration (microporous membranes) and the controlled formation of nanostructured solids for bioencapsulation and drug delivery. The methods of characterisation are X-ray Crystallography, NMR, Mass Spectrometry and vibrational spectroscopies, as well as EXAFS to assess the results of using different organic precursors (alkoxides, beta-diketonates and carboxylates).

Position in the area

Kessler has been active in the scientific community in terms of attending and organising conferences, his publication record (28 between 2006 and early 2008) and his collaborations. It is laudable that he has integrated the agricultural theme into his research programme. There are other indicators that Kessler has been successful in his research and in terms of educational impact. He has received (2003) the International Donald Ulrich Award for Excellence in Sol-Gel Science and is a member of the Advisory Board of the *Journal of Sol-Gel Science and Technology*.

Particular achievements

Kessler's fundamental synthetic studies of metal alkoxides has led to the realisation that many previous notions about these systems are not, in fact, entirely tenable. Metal Alkoxide Chemistry is over 100 years old and certain firmly embedded tenets regarding the nature of these compounds have somewhat hampered the development of the field. Kessler's one-pot, self-assembly approach may prove generally useful. He views the metal alkoxides as salts and uses the radius–ratio rule to predict products — a strategy he calls the 'Molecular Structure Design Concept' (MSDC). Kessler has two patents on the preparation and use of metal alkoxide precursors.

Future prospects

Project plans

During the interview Kessler presented his plans to implement sol-gel-derived materials in bioapplications, such as implants, and seed encapsulation. In his written report, he also states that he is planning to develop precursor-based approaches to catalytic membranes for photochemical water purification, separation of components in conversion gas (application with European Institute of Membranes and ECN) and catalytic membranes for low-temperature oxidation and metathesis (collaboration with BASF, Germany).

The goal of gaining (within five to ten years) an understanding of the connection between precursor properties and pore size (and pore-size distribution) in microporous membranes and the transport and catalytic

properties, if achieved, would be a helpful contribution. It is the expert panel's opinion that mastering the art of preparing chemically uniform crystalline nanoparticles should be given higher priority than it appears, from the presentation, to enjoy at present.

Balance between resources and goal

Past performance warrants continued funding.

Comments on the area

Position in Inorganic Chemistry

The area of precursor chemistry is central to the interests of the inorganic community. Kessler's research is evidently being published in standard, high-profile Inorganic Chemistry journals.

Importance of the area

Sol-Gel Chemistry has existed for quite some time, as has Molecular Precursor Chemistry, but they remain important disciplines for materials design and synthesis. Although a fair amount of this research often ends up in the hands of chemical engineers and others whose interest is purely technical, it is imperative for chemists to continue to take a leading role in tackling the issues of the relationship between precursor structure and materials structures and properties, as well as the mechanisms by which precursors evolve into materials. In particular, molecular precursors to oxides have many applications and oxide nanocrystals with well-defined distributions prepared from micelles would be a major contribution to the field. Kessler looks set to make this happen with the rational design methodology he is developing and should consider pursuing this angle.

Future potential of the area

Although it is very much a matter of classic Coordination Chemistry (as pursued by Don Bradley in the 1950s) there is certainly, given the applications in Medicine, Agriculture and catalysis, potential for growth in the area — especially through chemists' collaboration with engineers and the medical community. It was particularly interesting to see how Kessler encapsulated microorganisms and then monitored their release.

Overall assessment

Kessler's research is rated *very good* by the panel and continued funding is *strongly recommended*.

Lars Kloo

Division of Inorganic Chemistry, Department of Chemistry,
Royal Institute of Technology

New media for clusters, low-dimensional materials and electrolytes

Summary of the research programme

This research emphasises three topics: synthesis, structure and bonding, with special emphasis on p-block elements and an occasional excursion into the d-block. Two different projects funded by the Swedish Research Council are reviewed, First, new reaction media are being sought for the stabilisation and isolation of subvalent bismuth clusters, organometallic complexes and low-dimensional solids. Second, new ionic liquid electrolytes are being developed for photoelectrochemical solar cells. New organic cationic components have been investigated with the aim at removing viscosity and/or diffusion limitations of the ionic liquid electrolytes known at present.

Past performance

Methodology

A sizable effort is devoted to synthesis, complemented by a suite of characterisation techniques including X-ray crystallography, vibrational spectroscopies and other spectroscopies. Most recently, Lars Kloo has become interested in Bioinorganic Chemistry and brought methods relevant to this interest, including large-scale molecular dynamic computational methods for biomolecules, into his laboratory.

Position in the area

Kloo has developed a very interesting line of research centred on the subvalent bismuth cluster compounds. He has embarked on a new venture on solar cells, working closely with some of the leaders in the area (such as Anders Hagfeldt at Uppsala University). Kloo has been highly productive over a broad area of Chemistry, including setting up some valuable collaborations.

Particular achievements

Reaction chemistry has been devoted to electron-poor (group 15) and electron-rich (group 17) p-block elements. Several interesting subvalent bismuth and related clusters were prepared with gallium cluster anions.

The key to obtaining the subvalent bismuth clusters was the use of a GaX_3-arene (X=halide) solution mixture. The use of the gallium halide permits extremely high concentrations (50% solubility) of the putative anion to be achieved in benzene solutions. In addition, the gallium halide counter-anions are sufficiently stable to effectively 'trap' the bismuth cluster cations. Kloo has introduced transition-metal species into the mix and obtained some truly fascinating compounds. The expert panel particularly approved of a dimer of Pd(I) atoms bonded to a benzene ring. The work is akin to research in Japan that also involves placing strings of metal atoms under an arene canopy. Over time, this research may very well establish a new area of Organometallic Chemistry.

The efficiency of Grätzel cells is limited by the open-circuit voltage established by the I_2/I_3^--couple and the nitrile solvent, which limits the overall long-term value of these cells. Kloo has sought to replace this volatile organic solvent with ionic liquids.

Future prospects

Project plans

Synthesis of novel subvalent, organometallic and low-dimensional solids will continue to be a flagship of this research. The work on solar cells will turn to discovering an ionic liquid as an electrolyte that possesses low viscosity. This is logical and success in this area will represent a major contribution to the area of solar cells.

Balance between resources and goal

The balance at the Royal Institute of Technology (KTH) appears to be in grave jeopardy owing to problems relating to the flow of funds at University level. The faculty is under duress, with the need to raise money for members' salaries. This obliges them to pursue endeavours (professional and research) that will ensure that they receive their salaries. These endeavours are distracting the faculty at both the teaching and the research level. In the present case, a leading faculty member at KTH is unable to devote his attention to KTH because of having to pursue a variety of research options to secure a funding base for his salary. In so doing, Kloo is diluting his research effort: owing to the university's insufficient resources, he is pursuing areas of science that are incongruent with his goals.

Comments on the area

Position in Inorganic Chemistry

Kloo's synthesis of subvalent clusters makes him somewhat unique in Chemistry. Many people are working on the electrolyte problem in solar cells. However, by virtue of his collaboration with Hagfeldt, Kloo is in a strong position to exert an impact in this area.

Importance of the area

One distinctive talent of chemists is that they can make new combinations of matter. In Kloo's case, these are subvalent cluster compounds.

Future potential of the area

Synthesis of new compounds is powerful. Their utility is invariably unknown at the time of creation, but — within years or in decades — the compounds often find important new applications. The ability to make new compounds will always occupy a central position in science.

Overall assessment

Kloo is recommended not to dilute his efforts unduly. His main interest is the synthesis of novel coordination and organometallic compounds. Because of the salary issue, he is being forced to undertake a wide range of research unrelated to the aforesaid research areas. Flitting from project to project, as he is obliged to do, detracts from the teaching and research mission of a very talented scientist. KTH needs to address the issues surrounding the funding of faculty salaries. Neglect of this concern is severely undermining the excellence of KTH.

Kloo's research is rated as *excellent* by the panel and continued funding is *most strongly recommended*.

Sven Lidin

Department of Physical, Inorganic and Structural Chemistry, Stockholm University

Intermetallic Chemistry

Summary of the research programme

Intermetallic compounds have attracted attention for their unusual bonding and structural properties. An improved understanding of these features and complex systems requires a very fundamental approach. Fairly recently, it has become clear that there is a natural focus of interest on investigating complex intermetallics, from a structural point of view and in terms of thermoelectric applications. A good thermoelectric material should be an electronic conducting crystal and yet a phonon glass. These requirements are well met in interstitial Zintl phases and in certain incommensurately modulated structures. Quasicrystals, too, may be target compounds for thermoelectric materials. The research deals with the synthesis and characterisation, measurement of physical properties and theoretical treatment of a number of systems of fundamental interest to the area of intermetallics, and shows promise with respect to thermoelectric applications.

Past performance

Methodology

The studies of quasicrystal approximants and incommensurate structures represent extremely challenging topics in Crystallography and Inorganic Structural Chemistry. Sven Lidin is working on interesting types of compound with potential applications as thermoelectric materials. In these, order-disorder phenomena, complex stacking features or nanostructuring (nanoprecipitates) frequently play a key role.

Position in the area

Lidin has an internationally well-recognised position as one of the leading inorganic chemists and crystallographers in the field of incommensurate structures and quasicrystals. He collaborates closely with other leading international groups in these areas, both on the experimental side and in methodological development.

Particular achievements

Lidin's structural studies of quasicrystals, as well as his studies of ordering schemes in systems with hexagonal symmetry, are of very high quality. Highly interesting knowledge of Structural Chemistry is obtained for highly complex Zn-Sb phases that show promising figures of merit with respect to thermoelectricity.

Future prospects

Project plans

Understanding of complex crystal structures of intermetallics and methodological competence will be further enhanced by further study of quasicrystals and incommensurate structures. The research will focus both on in-house issues, primarily intermetallics with potential application as thermoelectrics, and on challenging structural issues raised by international partners. Future plans include an intention to see a stronger combination of synthetic work (pure and doped compounds), property measurement and theoretical work.

Balance between resources and goal

The objectives are highly challenging and there should be sufficient funding for securing a good balance between staff resources for making novel intermetallic compounds, characterisation, measuring physical properties and theoretical work. The research has access to very good infrastructure and benefits from excellent international collaborations.

Comments on the area

Position in Inorganic Chemistry

Intermetallics, Zintl phases and pnictides are broad and important categories of inorganic compounds and materials. An understanding of their crystal structures is essential for a grasp of structure–property relationships on which to base the search for novel and improved materials. The studies of incommensurate structures and quasicrystals, as well as the methodology for describing structures in higher dimensions, represent interesting and emerging areas of Structural Chemistry and Crystallography. Several well-cited publications by the group have appeared in high-ranking journals.

Importance of the area

More and more technologically important inorganic materials have intricate crystal structures, exhibit phase transitions and have complex phase relations. Developing cutting-edge expertise in tackling complex inorganic

structures is therefore important for materials of this type and for Inorganic Chemistry and materials research. Developing improved thermoelectric materials and providing a basic understanding of principles governing their properties are vital endeavours in Materials Chemistry and Energy Technology.

Future potential of the area

There is ample potential for further high-quality research in the fields of quasicrystals, incommensurate structures and thermoelectrics.

Overall assessment

Detailed descriptions of complex crystal structures are a prerequisite for design and understanding of structure–property relationships of the utmost importance for many categories of advanced materials. In this respect, there is a strong need to maintain and further develop competence in analysing large superstructures, incommensurate structures and quasicrystals. Such knowledge is, moreover, important for an understanding of many novel types of thermoelectric material. Lidin combines advanced Crystallography with the study of key issues in Materials Chemistry. His research is rated as *excellent* to *outstanding*. Continued funding is *most strongly recommended*.

Jan-Olle Malm

Division of Polymer and Materials Chemistry, Department of Chemistry, Center for Chemistry and Chemical Engineering, Lund University

Nanocrystallography based on electron microscopy methods

Summary of the research programme

The present project focuses on solving crystallographic and structural problems on the nanometre level, using local analytical techniques. The work will provide tools to address such issues as local structure in grain boundaries, interfaces and nanoparticles. This will help to afford an understanding of growth processes and properties in these materials.

The project seeks to develop and implement techniques to enhance information in high-resolution transmission electron microscopy (HRTEM). This will ensure that the National Center for High Resolution Electron Microscopy (nCHREM) in Lund can compete internationally with leading laboratories in this field. Image reconstruction techniques for HRTEM and quantitative image matching will make it possible to improve information retrieval from high-resolution micrographs, which will in turn improve resolution of the 300 kV FEG-TEM in Lund, from a nominal structural resolution of 1.7 Å to close to 1 Å.

The ultimate goal is to create a user-friendly interface for focal series reconstruction, tilt-azimuth restoration and quantitative image matching, to ensure that the methods can be used on a routine basis for high-resolution work at nCHREM.

The project also has a basis in electron microscopy, in this case complemented by preparative Nanochemistry. The work involves preparation of tailor-made nanoparticles, followed by their characterisation both in the deposited form and in solution using cryo-TEM.

Past performance

Methodology

Jan-Olle Malm's project is focused on solving crystallographic and structural problems on the nanometre level using local analytical techniques.

Particular attention is devoted to developing and implementing techniques to enhance information in HRTEM. Thus, the cryo-HRTEM technique has shown atomic resolution for nanoparticles in solution.

Position in the area

Malm collaborates extensively with Swedish physicists from the Nanometer Structure Consortium in Lund and with an Oxford University group that provides Chemistry expertise in joint projects.

Particular achievements

Malm has concentrated on crystallographic analysis of III-V nanowires and of seed particles that catalyse growth. This analysis includes structure, phases and composition of the seed particles and affords a more profound understanding of the properties required for growth.

Future prospects

Project plans

The plan is to ensure sufficient knowledge and expertise to compete internationally within the areas of Materials and Structural Chemistry. Malm wishes to play an important part in developing new nanostructures. Today, we can only guess at future applications in this field.

Balance between resources and goal

The infrastructure supported by this grant has been important in the state-of-the-art workings of electron microscopy. The grant was awarded only recently, and one PhD student has been working on the project.

Comments on the area

Position in Inorganic Chemistry

Malm has adopted a position in which he supports the physical community of the Nanoscience Consortium, especially in characterisation of nanowires.

Importance of the area

Nanoscience is highly important. However, the application of scanning electron microscopy alone may appear to be more of a technical service than an area of scientific significance in its own right.

Future potential of the area

This area is expected to remain important in the future.

Overall assessment

Malm is running an impressive project, albeit one at risk of being considered part of the Physics Department. The research is rated as *very good*. Continued funding is *strongly recommended*.

Ebbe Nordlander

Division of Chemical Physics, Department of Chemistry, Center for Chemistry and Chemical Engineering, Lund University

Biomimetic/bioinorganic and organometallic chemistry of transition elements: synthesis and reactivity studies of mono- and polynuclear transition metal complexes

Summary of the research programme

The research project in Coordination Chemistry concerns Biomimetic and/or Bioinorganic and Organometallic Chemistry. The objective is to use transition-metal complexes as models for biological and industrial catalysts. The bioinorganic research is aimed at achieving better understanding of the physicochemical nature and reactivity of metal centres in biological systems. To correlate the reactivity of metallobiosites with their structural, electronic and chemical properties, new complexes are prepared that may emulate structural and/or functional properties of metalloproteins. Synthesis of biological cofactors and designed metalloproteins is attempted.

The research in Organometallic Chemistry concerns (i) development of chiral transition metal complexes that may be used as stoichiometric reagents, or as catalysts in asymmetric organic synthesis, and (ii) study of interactions between transition metal carbonyl and/or chalcogenide clusters with sulphur-containing compounds. The aim is to study the coordination modes of the organic ligands and to investigate whether their reactivities are affected by coordination to transition metal clusters. How such phenomena relate to industrially important reactions in both homogeneous and heterogeneous catalysis is explored.

Past performance

Methodology

The most important experimental method employed in the research is ligand design, followed by synthesis and characterisation of metal complexes, including single crystal X-ray diffraction.

Position in the area

Ebbe Nordlander is preparing a large variety of relevant and interesting coordination and organometallic compounds. His biomimetic work involves the majority of his group and has a recognised profile in the community, as his publications, collaborations and international visitors clearly show.

Particular achievements

Nordlander's activities concern two extensive and somewhat related topics, both associated with transition metal Coordination Chemistry and ligand design. He has had regular publications in high-ranking journals on most of the subtopics studied. Most recently, Nordlander's work on structural and functional modelling of dinuclear metalloproteins and his preparation of a diiron complex capable of oxidising hydrocarbons have attracted attention.

Future prospects

Project plans

Nordlander plans to continue to explore the various current subtopics in Bioinorganic and Organometallic Chemistry. This may appear ambitious. Accordingly, if the Swedish Research Council's funding is to remain as limited as it has been to date, the panel recommends focusing on a few of these topics rather than attempting to pursue them all. The work in the bioinorganic topics appealed most to the expert panel, although Nordlander is certainly highly qualified to address the organometallic topics as well.

Balance between resources and goal

To date, the research has entailed a relatively small staff effort, involving only a few PhD students supported by the Swedish Research Council. Nordlander has good ideas and plans, as well as the capacity to manage a larger group. Extension of the funding should be considered and is most strongly recommended by the panel. Since the work is not performed in an Inorganic Chemistry department, attention should also be paid to funding for crucial equipment, such as that required for X-ray crystallography.

Comments on the area

Position in Inorganic Chemistry

Nordlander is operating in an important subarea of Inorganic Chemistry, where he has earned a well-recognised international position. He has also contributed to this community with a number of well-written reviews in recent years.

Importance of the area

Internationally, the area of biomimetic, bioinspired Coordination Chemistry is large and still growing. Nordlander is one of the very few scientists from Sweden active in this field.

Future potential of the area

The broad field of Coordination and Organometallic Chemistry, with subtopics in, for example, Biomimetic Chemistry and homogeneous catalysis, is likely to remain a major area worldwide for the next decade at least, and should be studied in Sweden as well.

Overall assessment

Nordlander has designed and prepared several very interesting biomimetic and organometallic compounds. The panel believes that, in the long run, Nordlander's research will benefit from some concentration on the strongest topics. His science is better than that of some professors, and the panel finds it somewhat unusual to see such a creative and productive researcher who has not yet been promoted. The overall quality of his research is rated as *very good* to *excellent*. Continued funding from the Swedish Research Council, with an increase in grant size if possible, is *most strongly recommended*.

Ingmar Persson

Department of Chemistry, Swedish University of Agricultural Sciences

Structure, bonding and thermodynamics of metal ions, anions and complexes in solvents with special properties at coordination

Summary of the research programme

The research focuses on the influence of solvents on such physicochemical properties as solubility, redox and distribution equilibria, stability of complexes, reaction rates and mechanisms, and spectroscopic and structural properties. The chemical properties of most metal ions in aqueous solutions are well known. The focus here is on how different solvents can affect structures and properties. Reactions in liquid ammonia and N,N-dimethylthioformamide, and in the bulky N,N'-dimethylpropyleneurea (DMPU) solvent molecule, were investigated. The main issues addressed are the nature of hydration and solvation for groups 5–13 and lanthanide(III) metal ions and the nature of hydration for anions in aqueous solution. Another line of investigation is the study of complex formation in solvents where the metal ion adopts a lower coordination number than in water for electronic or steric reasons.

Past performance

Methodology

The principal methods used are EXAFS, XANES, metal NMR spectroscopy, crystallography, calorimetry, potentiometry and mass spectrometry. Owing to the multidisciplinary nature of the work, experiments need to be conducted at other labs, including the synchrotron facility at MAX-lab. This project is being conducted in close collaboration with groups at Stockholm and Linköping Universities, the University of Rome, the Technical University of Gdansk and the Polish Institute of Nuclear Chemistry and Technology in Warsaw.

Position in the area

Ingmar Persson is involved in methodological development of several important techniques for characterising complex mixtures and other materials for which crystallography data are unavailable or fail to give a complete structural picture. These are High Energy EXAFS (with energies >40 keV), sulphur XANES and Large Angle X-ray Scattering (LAXS). He is to be commended

for helping to popularise these techniques in Sweden. He has mentored a large number of PhD students, including a few faculty members at universities in Sweden. He is evidently highly regarded in the community in Sweden, thanks to his own research, which has been published in high-ranking peer-reviewed journals, and his teaching. He is also fairly active in the community, judging from his participation in top international conferences.

Particular achievements

One key result is from the structural determination of the hydrated lanthanide(III) ions in solid state and aqueous solution, all with tricapped trigonal prismatic configuration. The heaviest ions, Ho-Lu, have an increasing tendency to lose water molecules in the capping positions, in both solid state and solution. An explanation for this situation, which is referred to as 'broken coordination', has been provided. The conclusion is that the 'gadolinium break' has no structural roots, except possibly a hydrogen-bonding one. The Sc(III) ion behaves like an extreme case for the heavy ions in the 4f series. Their structures provided a viable explanation for their catalytic properties involving C-C bond formation in aqueous media. The hydrated palladium(II) ion was found to be six-coordinate with weakly axially coordinated water molecules, approximately 0.7 Å longer than the equatorial ones. This helps to explain many of the substitution reactions of Pd(II). Hydrated Ca(II), Zr(IV) and Hf(IV) ions are all eight-coordinate in a square antiprism arrangement. The hydrated Ag(I) binds two water molecules more strongly than the remaining two to four water molecules in a distorted arrangement.

DMPU, an aprotic solvent with strong electron-pair oxygen donor properties, is quite bulky in its coordination to a metal ion. Five-coordination is observed, rather than octahedral solvates, and the reactivity of the metal ion is substantially higher for these less stable solvates.

Future prospects

Project plans

Persson's plan is to continue with his present activities with more emphasis on the hydration of anions, which have been little studied owing to inherent experimental difficulties. More work on Coordination Chemistry on DMPU, a sterically demanding solvent, will also be carried out. In general, it appears that the lines of research already being pursued will form the basis for future efforts. Although simple systems are suitable for testing theories and models, the expert panel suggests tackling larger problems. For example, given the lack of knowledge of many aqueous systems in nature, applying the tech-

niques used and mastered in this lab to Biology and Environmental Sciences would be beneficial.

Balance between resources and goal

The funding from the Swedish Research Council and from the Swedish University of Agricultural Sciences for Persson and his research appears to be adequate for the current efforts (with help from other grants for post-doctoral researchers). The synchrotron time needed to carry out the research is substantial, and obtaining the necessary beam time does not appear to have been a problem. If more resources were made available, it would probably exert most impact if Persson could engage a senior person who could provide long-term expertise for the students and postdoctoral researchers in the areas of LAXS, high-energy EXAFS etc.

Comments on the area

Position in Inorganic Chemistry

The use of high-energy spectroscopic techniques for the chemical problems represented by this research is not typical or limited to Inorganic Chemistry, but such fundamental studies can have far-reaching implications if applied to Biology and Materials Chemistry.

Importance of the area

High-energy EXAFS, LAXS and sulphur XANES, in particular the latter, are extremely important techniques for use in Inorganic Chemistry.

Future potential of the area

The development of sulphur XANES would be very useful for probing metal sulphur clusters in proteins. In general, the tools used in this research can be used to reveal information about many types of compounds and materials.

Overall assessment

The research being carried out by Persson is of high quality and his several collaborations are proceeding very well. The research is rated as *excellent* and further funding for this research is *strongly recommended*.

Per Persson

Department of Chemistry, Umeå University

Coordination Chemistry at the interface between aqueous solutions and micro- and nanosized metal-oxide particles

Summary of the research programme

The research led by Per Persson in the Aquatic Chemistry Group in the Chemical Biological Centre at Umeå University is an interdisciplinary effort aimed at integrating Inorganic Chemistry with environmental research. The rationale of the research is that nearly all environmental problems involve interfaces of water-based species with naturally occurring solids. One theme is 'Processes and Mechanisms', which encompasses the issues of adsorption, composition, stabilities and structures of surface species, as well as desorption rates and/or mechanisms and surface catalytic processes. A second major theme is 'Sample Characteristics and Origin', which focuses on speciation of elements in natural samples, reactivity of natural solutions and solid matrices, as well as organic and inorganic molecules and fundamental studies at water–solid interfaces. Most of the work presented has covered the last subtopic. All the issues tackled concern fundamental aspects of Surface Coordination Chemistry. The research covers both well-characterised surfaces of crystalline particles and water-soluble metal-oxide clusters. The clusters serve as an important link in the chain from mononuclear complexes to complexes of nanosized particles and larger (micron-sized) crystalline particles. The main objectives of the research are to characterise, at the molecular level, the structure, bonding and reaction mechanisms of inorganic and organic ligands, metal ions and metal-ligand (ternary) complexes on metal-oxide particles and with metal-oxide clusters in aqueous solutions. The ultimate goal of these investigations is to understand structure–reactivity relationships: the interplay between the structures of the interacting species and the metal-oxide surface respectively.

Past performance

Methodology

The systems described are characterised by means of synchrotron-based EXAFS and XANES, photoelectron spectroscopy and vibrational spectroscopy. Theoretical modelling of EXAFS and XANES spectra and theoretical

vibrational-frequency calculations are performed to support interpretation of experimental data. This research provides fundamental, molecular-scale information that enhances the understanding of and ability to exploit surface reactions on metal-oxide particles and clusters. In tandem with Persson's research efforts are the companion studies of his collaborator, Professor Staffan Sjöberg, who provides information on complex, pH-dependent equilibria occurring at the mineral surface during reactions involving organic ligands, external metal ions and, in some cases, soluble components of the mineral itself. By pooling their expertise, the two groups are piecing together valuable models for extremely complicated chemistry that may arise under different environmental conditions. The work is divided between the Persson group and the Sjöberg group as follows: Persson extracts structural and electronic information by the application of spectroscopy under various conditions of equilibrium and non-equilibrium conditions, and Sjöberg uses his knowledge of solution chemistry to work out the details of composition, stability, kinetics and mechanisms.

Position in the area

Persson is a highly competent, extremely productive researcher who, with his collaborator and as a sole author, has published well-cited articles in a variety of journals, many of which (for example, *Langmuir*) have a high profile in the area. Given his ties with Biogeochemistry and Ecology as well, he can move easily among communities. At the same time, there is no doubt that the Inorganic Chemistry he is doing is basic and fundamentally important.

Particular achievements

Molecular-level adsorption mechanisms for organic acids at the water–mineral interface were studied and surprising findings emerged. Previously, the generally accepted idea was that organic acids containing carboxylate functional groups form contact-ion pairs or inner-sphere complexes at water–metal hydroxide interfaces and that, accordingly, direct bonds are formed between oxygen atoms of the carboxylate groups and the surface metal ions. By combining wet-chemical methods, ATR-FTIR spectroscopy and molecular orbital calculations, Persson and his collaborators have shown that carboxylic acids form both inner-sphere surface complexes and outer-sphere hydrogen-bonded complexes. The data indicate that the balance between inner- and outer-sphere surface complexes is influenced by such factors as solution pH, structure and composition of the organic acids and the surface. They also show that certain inner-sphere surface complexes may be thermodynamically stable entities, and not necessarily transition

states in dissolution pathways as previously suggested. These results have altered the manner in which ligand-promoted dissolution phenomena are viewed, which has a major bearing on nutrient dynamics in soils and aquifers. These findings have triggered a number of studies on dissolution processes by other research groups.

Future prospects

Project plans

Persson plans to focus on the molecular biogeochemistry of P and Fe, and in particular to further strengthen his collaborations with ecologists and soil scientists. The projects that have been initiated, such as 1) ligand competition effects between organic acids and orthophosphate at the water–mineral interface and 2) abiotic and enzymatic hydrolysis of organophosphates in aquatic and terrestrial environments, will be continued. Persson and his group also plan to engage a postdoctoral researcher to carry out P-NMR spectroscopy for the phosphorus projects. Molecular characterisation of Fe in natural samples by means of synchrotron radiation is also planned. These are ambitious efforts that will require more coworkers, especially a permanent staff member to focus on synchrotron research.

Persson plans to expand his endeavours in Coordination Chemistry at the water–solid interface, which has seen less activity in the past few years owing to lack of time. The plan is to step up future funding and research efforts in this area, in particular the dynamic aspects of the reactions and complexes. The team has recently developed an ATR-FTIR spectroscopic probe, permitting studies of the labilities of surface complexes, which will be very useful for these studies. The need to acquire another FTIR spectrometer and upgrade the Raman equipment was stressed.

Balance between resources and goal

In 2007, when the Chemistry Department was reorganised, Persson returned as a Professor. His current position involves 75% research and 25% duties as deputy head of the department. His intention is to increase his activities in Coordination Chemistry at the water–solid interface. Since this work is very important and intimately bound up with the field of Biogeochemistry, returning to the fundamental studies is perceived as highly relevant. In the future, however, it will be important to find a successor to his collaborator, Staffan Sjöberg, who will be retiring soon.

Comments on the area

Position in Inorganic Chemistry

The Chemistry Department at Umeå University has been reorganised in three divisions: Biological, Environmental and Technical. Persson has very neatly integrated Inorganic Chemistry with his responsibility for 'Aquatic Chemistry', which is a highly relevant area of Inorganic Chemistry.

Importance of the area

This is a fascinating application of Chemistry and sustainability. With our planet's changing face, work in Chemistry such as Persson's will continue to grow in importance in the future. There will be a host of problems in Inorganic Chemistry that, with our increasing environmental awareness, need solving. Examples are the growth of biofilms due to siderophore transport and bacteria that use iron as an external metabolite for mitochondrial energy generation. The mechanisms of these processes are fascinating, and excellent inorganic chemists like Persson can help us to understand the processes.

Future potential of the area

With an increased awareness of our planet and the role Chemistry will play in sustainability, Persson is already poised to address future challenges in the field.

Overall assessment

Persson is an excellent example of how a professor in Sweden whose background is in Inorganic Chemistry can take advantage of the opportunities on offer to carve out an exciting frontline career. Chemistry at the Chemical Biological Centre at Umeå University has been reorganised into three divisions, including the Aquatic Chemistry group of which Persson is a member. This administrative change appears to have been a success. The expert panel rates Persson's research as *excellent*. Continued funding is most *strongly recommended*.

Magnus Sandström

Department of Physical, Inorganic and Structural Chemistry, Stockholm University

Coordination and chemical bonding in solvated complexes and ions, especially by means of X-ray absorption

Summary of the research programme

Structural and spectroscopic determinations, in combination with theoretical calculations, are used for systematic investigations of various types of chemical bonding for hydrated and solvated metal ions and complexes, preferably for species in solution without packing effects. Many chemical properties of molecular species depend on a complex interplay between size and the electron distribution of the central atom, and the electron-donating properties of the ligands and their steric interactions. Sulphur compounds of importance for natural systems are also being studied. One powerful tool is synchrotron-based X-ray absorption spectroscopy (XAS), where the fine structure after the absorption edge (EXAFS) is used for lattice-independent studies of the local structure around the absorbing atom, while the electronic transitions at the absorption edge (XANES) can be used to yield information on its oxidation state and characteristic surroundings. At the sulphur K-edge, the intense synchrotron X-ray radiation at beamlines in SSRL in the USA, and used for microspectroscopic mapping in ESRF, France, makes it possible to study transformation and accumulation of sulphur compounds in wood, soil and sediments, even for intact natural samples. The methods of analysing the sulphur K-edge XANES spectra are being developed by means of both theoretical calculations and empirical speciation analyses. The results have a bearing on sulphur accumulation processes and transformations in natural samples, such as marine-archaeological wood, and on uptake of reduced sulphur compounds in kerogens (fossil fuels) through reactions with lignin in humic matter contained in marine sediments.

Past performance

Methodology

Structural and spectroscopic determinations in combination with theoretical calculations elucidate various types of bonding for hydrated and solvated metal ions and coordination compounds, preferably without packing effects. Electron-donating properties and their steric interactions are described. Sulphur compounds of biological interest are studied. XAS, EXAFS, and XANES are used to characterise the oxidation state and immediate surroundings.

Position in the area

Magnus Sandström is a world leader in the field of Structural Analysis methods. In addition, he is an undisputed leader in Cultural Heritage Sciences, as his analysis of sulphur in old shipwrecks, for example, shows. Sandström is also an authority on solvation of rare earth-metal ions, and he is thus carrying Swedish traditions in this area to the cutting edge.

Particular achievements

Sandström's discovery and the marine-archaeological consequences of sulphur accumulation in wood of historical shipwrecks have attracted worldwide attention. This work has been referred to in the daily press, such as the *New York Times*, *Washington Post*, *Die Welt* and such popular science magazines as *Scientific American* and *New Scientist*. In this connection, he has given numerous lectures.

Future prospects

Project plans

Scientists from all over the world stand in line to collaborate with the group, which should keep it busy for a long time to come. The extensive machine park involved in Sandström's operations is relatively new and only a solid-state NMR seems close to needing an upgrade. Thus, the two lines in the present scientific work are expected to continue.

Balance between resources and goal

The running cost for the machines is high and may even increase if liquid-helium prices rise. Considering the scientific output and the number of PhD (six) and MSc (one) students receiving education within Sandström's research, the expense is more than justified.

Comments on the area

Position in Inorganic Chemistry

Sandström's work on solvation of rare earth ions and structure analysis is central to Inorganic Chemistry. It involves many different techniques and the group's expertise covers them all. The exciting work on degradation of wood in old shipwrecks is of immediate public interest and adds glamour to Inorganic Chemistry, which seems much in demand right now.

Importance of the area

The highly academic investigations of coordination numbers for lanthanides that have recently been conducted are also, in fact, important in view of metal ions in Medicine. These metal ions include some with high magnetic moments that are used in treatment or scanning methods. Ligands allowing these metal ions to enter the bloodstream are designed partly in response to results based on measurements of coordination number.

Future potential of the area

X-ray techniques for the study of solvated complexes and ions will remain highly relevant not only for the inorganic chemists but also for the more general scientific community.

Overall assessment

Sandström is highly successful in both of his two major research areas, and the expert panel also commends his vigorous efforts to show the public how important basic science is in solving practical problems. The research is rated as *excellent* to *outstanding*. Continued funding is *most strongly recommended*.

Staffan Sjöberg

Department of Chemistry, Umeå University

Chemical speciation in solution and at solid–solution interfaces. Models and modelling

Summary of the research programme

The research in this project, undertaken in collaboration with Professor Per Persson, involves the study of chemical transformations that take place at solid surfaces and of interfaces in aqueous systems. Detailed molecular structure data (Persson) combined with macroscopic measurements (Staffan Sjöberg) are being used to develop models that describe the thermodynamics, kinetics, structure and reaction mechanisms of interfacial processes. The systems studied range from well-characterised small model systems, from Ångström level clusters of anionic and cationic polyoxometallates to nanometre- and micrometre-sized particles of different metal oxides and hydroxides. The various cluster systems are studied vis-à-vis surface protonation and deprotonation and the adsorption of metal ions, for the purpose of comparing the results with metal-oxide and hydroxide minerals. The ultimate goal is to feed all the information into a model that attempts to explain and predict speciation by using recently developed models, including electrical double-layer theories that allow mechanistic multilayer, multisite descriptions of the solid–water interface.

Past performance

Methodology

This research seeks to afford an understanding of chemical speciation at the solid–solution interface. Interaction of various ligands with mineral surfaces is studied by monitoring species concentrations at various pH values by means of potentiometric titrations. The techniques employed are numerous and include FT-IR, FT-Raman, EXAFS and XPS, as well as potentiometry, voltammetry, adsorption studies and z-potential measurements. One example of a typical study is the chemistry at the solution–goethite interface. A sample of a well-crystallised mineral is used and a suspension of the mineral is subjected to various chemical environments. An interplay of connected reactions arises with the addition of an organic ligand, such as a glyphosate, which can bind to the surface of the mineral. Competition

studies are then performed by the addition of a metal ion, which leads to complex equilibria. If the mineral is also capable of being dissolved at certain pH values, the system is even more complex. This is true of hydroxyapatite, which releases phosphate ions.

Position in the area

This collaborative research is highly relevant to today's environmental and ecological issues, and the Sjöberg–Persson team is somewhat unique among inorganic chemists. The work is divided between the Persson group and the Sjöberg group as follows. Persson extracts structural and electronic information by applying spectroscopy under various conditions of equilibrium and non-equilibrium, and Sjöberg uses his knowledge of Solution Chemistry to work out the details of composition, stability, kinetics and mechanisms. The reorganisation of the Chemistry Department at Umeå University has been highly successful, judging by this pair of researchers in the Aquatic Chemistry group.

Particular achievements

Three minerals — goethite, alpha aluminium oxide and manganite — were studied in different ligand environments, including phosphono-methylglycine (PMG), with three donor groups: a phosphonate, an amine and a carboxylate group. Data reveal that PMG adsorbs to the surfaces of these minerals via one oxygen atom of the phosphonate group. Coadsorption of PMG and Cd(II) on the surfaces of goethite and manganite was found to result in the formation of binary and ternary mineral-PMG-Cd(II) surface complexes.

Dissolution and surface complexation of hydroxyapatite (HAP) and fluorapatite (FAP) were investigated with a combination of different techniques, and models were generated to explain the dissolution and surface-complexation properties. Specifically, it was found that both apatites form surface layers that deviate from their bulk compositions when they are equilibrated in aqueous solutions. The presence of goethite also enhances the dissolution of FAP as it reacts with the released phosphate and precipitates as iron phosphate, which alters speciation. This finding has implications for the bioavailability of phosphate in this two-mineral system.

Future prospects

Project plans

Sjöberg's grant from the Swedish Research Council expires at the end of 2009. In five years' time he will be a Professor Emeritus. He is currently involved in several PhD projects that are to be concluded in 2010 and he plans to continue acting as supervisor for these. At present there is no obvious successor with expertise in modelling in his department. This is unfortunate, since this research is important for supporting and complementing the efforts of Per Persson.

Balance between resources and goal

The funding has been adequate to meet the project needs, and the necessary facilities for carrying out the research are excellent and are likely to remain so in the future.

Comments on the area

Position in Inorganic Chemistry

This kind of Inorganic Chemistry may not be in the mainstream of global Inorganic Chemistry (or in part it may be regarded as Physical and/or Analytical Chemistry), but it is an important molecular topic. Many of the central problems that must be solved in the future, such as understanding the role of minerals in the chemistry of the environment, are essentially rooted in Coordination Chemistry, albeit in a fairly complex manner.

Importance of the area

A good deal of information appears to be available in the literature on the surface adsorption of various molecules on inorganic surfaces using macroscopic methods. In more recent times, new spectroscopic techniques for obtaining molecular-level surface structural data and the advent of new theoretical methods for studying hydrated interfaces have permitted a quantum leap in knowledge and opened up whole new avenues for understanding surface complexation. Unfortunately, it is typical for independent research groups to focus either on the macroscopic characterisation of adsorption processes or on the interpretation of surface processes at the molecular level. The Sjöberg–Persson research team is unique in that they are engaged in extremely synergistic activities that combine molecular and macroscopic information, thus allowing much more reliable surface-complexation models.

Future potential of the area

There is immense future potential for using the knowledge gained here to understand important problems in the environment, catalysis etc.

Overall assessment

The Sjöberg group's efforts over the years have paid off in terms of important advances in understanding the surface chemistry of important materials. Since he will be retiring soon, funding of a project related to this effort, which the expert panel rates as *excellent*, is *strongly recommended*.

Gunnar Svensson

Department of Physical, Inorganic and Structural Chemistry, Stockholm University

Synthesis and structural characterisation of nanoporous carbons and transition metal oxides

Summary of the research programme

Two projects have been supported by the Swedish Research Council: syntheses and characterisation of (1) carbide-derived carbon (CDC) materials and (2) cobalt-based perovskites.

Carbide-derived carbons (CDCs) have been prepared and characterised using gas adsorption, Raman spectroscopy, reverse Monte Carlo modelling using neutron diffraction data, scanning and transmission electron microscopy, and electron energy-loss spectroscopy. The structure of the CDCs has been adjusted by means of i) synthesis temperature, ii) carbide precursor, iii) the presence of catalysts, and iv) bulk density and the precursor. Varying morphologies of the CDCs are obtained under specific conditions, and CDCs have been obtained that are amorphous or nanoparticulate, depending on specific reaction conditions. Porosity of the materials as a function of CDC structure has been investigated.

Oxygen-deficient cobalt perovskites, $A_{1-x}B_xCo_{1-x}M_xO_{3-x}$, have been synthesised and characterised using X-ray and neutron powder diffraction in combination with high-resolution electron microscopy and electron diffraction. Electronic structure and the magnetic properties of these compounds have been investigated.

Past performance

Methodology

The CDC research depends on classic reaction of the chlorination of carbides under a variety of conditions. Knowledge of the synthesis conditions has been guided by thermodynamic calculations. The group excels in synthesis of transition compounds based on metal oxides and using diffraction techniques to guide the design of new materials.

The group relies on a palette of spectroscopic techniques to characterise new materials. Structural characterisation is accomplished with electron, neutron and X-ray diffraction techniques. Newly acquired expertise in electron energy-loss spectroscopy has been exploited for quantitative study of disordered carbons. Structural studies are supplemented by reverse Monte Carlo simulations. Raman spectroscopy has also been used for characterisation of CDCs.

Position in the area

Gunnar Svensson has been highly productive in both the CDC and the perovskite research project. In the expert panel's view, he is performing some fine research and would benefit from increased visibility at international meetings, by attracting international visitors etc.

Particular achievements

Svensson has defined synthesis conditions that yield CDCs with pore sizes ranging from micropores (at low temperatures) to mesopores at high temperatures. A correlation of pore-size distribution has also been defined. High-resolution spectroscopy has shown that the carbons preserve sp2-type hybridisation, and Svensson has proposed the interesting hypothesis that ring sizes become more uniform for six-membered rings with an attendant decrease in puckering.

Several new perovskites have been prepared, affording scope for very interesting magnetism and catalysis properties. Oxygen-deficient cobalt perovskites have been prepared and characterised using X-ray and neutron powder diffraction in combination with high-resolution electron microscopy and electron diffraction. Interesting structural-electronic correlations have been observed for some materials.

Future prospects

Project plans

The research on CDCs is to be terminated owing to resource constraints. Svensson will continue to work on cobalt perovskites with a view to their application as catalysts at the cathode of fuel cells.

Balance between resources and goal

This is a modest research group comprising two PhD students and one post-doctoral researcher. It is a group that makes heavy use of instruments and would benefit tremendously from a scientific-cum-technical staff member to help maintain instruments, train students in their use and design experiments. The funding level is seen as adequate.

Comments on the area

Position in Inorganic Chemistry

Recent work on carbon derived from metal-carbide precursors, the very field in which Svensson is working, has shown capacitance rising with expanding pore size beyond the dimensions of the solvation shell. Increases in storage capacity of as much as 50% above the best-performing commercially available activated carbons have been observed. Considering Svensson's expertise, he is capable of making a significant contribution to this very topical and important field in energy storage.

The work on cobalt peroxide is exactly the type of research that should be pursued under the Swedish Research Council. Svensson is using the funds from the Council to pursue fundamental studies aimed at discovering new materials for fuel-cell applications. In his work, he is achieving a rapid transition to fuel cells in a well-constructed collaboration.

Importance of the area

The work has two important design objectives: nanostructured porous carbon for a variety of applications and new cobalt perovskites for catalyst applications, especially oxygen reduction. Both areas are prominent research endeavours at the forefront of the subject of Chemistry.

Future potential of the area

CDCs are being examined as gas absorbents. This is a historic application of these materials. Svensson has begun to define the factors that control pore-size distribution in CDCs. It should be noted that recent years have seen a move away from carbon-based absorbents to more elegant materials with even better controlled pore sizes, namely the metal-organic frameworks (MOFs). The advantage of MOFs is the scope they afford for controlling pore size with extreme fidelity. To exert a major impact with CDCs, Svensson will have to show where his approach competes with more modern, designed solids.

Svensson may wish to monitor research on cobalt-deficient oxides that exhibit superconducting properties.

Overall assessment

Svensson has wisely transferred his expertise in Structural Chemistry to emerging areas in Inorganic Chemistry. He correctly identifies the need for new catalysts at the cathode of fuel cells and nanostructured carbon for a variety of applications in gas adsorption and supercapacitors. It is unfortunate that Svensson is to terminate the CDC project owing to constraints on group size.

The research is rated *very good* by the panel and continued funding is *strongly recommended*.

Jan-Erik Svensson

Environmental Inorganic Chemistry, Division of Energy and Materials, Department of Chemical and Biological Engineering, Chalmers University of Technology

Active corrosion of Fe-Cr alloys at high temperature: chemical breakdown of chromia-containing oxide scales by the formation of gaseous species

Summary of the research programme

The usefulness of Fe-Cr alloys in high-temperature applications relies on the formation of a protective chromia-containing oxide scale. In certain environments, (O_2+H_2O, HCl) the materials may fail to form a protective oxide, resulting in rapid corrosion. This effect has been the subject of much speculation. The project has revealed that chromia is vaporised from the protective scale of stainless steel at a temperature as low as 600°C in O_2+H_2O environment. This project addresses fundamental studies of chromia vaporisation and its effects on the corrosion behaviour of iron-chromium alloys. It represents concerted forces in Corrosion Chemistry, Solid State Chemistry, Microscopy and Theoretical Chemistry. Density functional theory (DFT) calculations are used to determine molecular structure and investigate the surface reaction. The consequences of chromia vaporisation on the composition and microstructure of the oxide and the effects on oxidation kinetics are studied. The microstructure is investigated using a combination of techniques, including TEM and FIB. The project has generated new insight into the chemistry and physics of oxidation. This is highly relevant in Materials Science, as well as to energy production. The project also addresses corrosion issues in combustion environments, such as power boilers using biomass. It therefore has a bearing on society's endeavour to achieve sustainable energy systems.

Past performance

Methodology

Jan-Erik Svensson focuses on high-temperature oxidation studies of FeCr and FeCrNi steels. Such steels have a bearing on, for example, biomass- and waste-fired boilers and solid oxide fuel cells (SOFC) applications (500–850°C). Chromium vaporisation is a key parameter for actual corrosion processes. The rate of Cr vaporisation and its influence is investigated as a function of gas composition, gas velocity and alloy composition. This includes, for

example, preparation of metal-oxide cross-sections by means of focused ion-beam milling for scanning and transmission electron microscopy investigations.

Position in the area

The Competence Center for High-Temperature Corrosion (HTC) at Chalmers University of Technology is internationally eminent in research on chromium vaporisation and high-temperature oxidation of FeCr and FeCrNi steels. The atmospheric corrosion research is of very high quality and uses state-of-the-art methodology.

Particular achievements

Degradation of FeCr alloys at high temperatures in an O_2+H_2O environment is caused by failure of the protective oxide. This is shown to be due to depletion in chromium(III) by oxidation to Cr(VI) followed by vaporisation as $CrO_2(OH)_2(g)$. This finding is supported by DFT calculations and experiments. Svensson has made important advances in mitigating this problem by modifying atmosphere and alloy composition.

Future prospects

Project plans

Svensson intends to continue his work on high-temperature corrosion and atmospheric corrosion, focusing on fundamental aspects. In high-temperature corrosion, the work will focus on the effect of water vapour and alkali salts, and on the effect of chromia vaporisation and chromate formation of iron-chromium alloys.

Balance between resources and goal

As part of a broader collaboration on high temperature and atmospheric corrosion at Chalmers University of Technology, adequate resources appear to be available to yield ample future advances in both the priority areas.

Comments on the area

Position in Inorganic Chemistry

High-temperature corrosion causes breakdown of many components and systems operating at high temperatures and in harsh conditions. A profound understanding of relevant corrosion mechanisms must necessarily involve knowledge and study of, for example, surfaces, gas species, diffusion and phase relations, which all involve important aspects of Inorganic Chemistry.

Importance of the area

Corrosion is an important area in applied Materials Science. The ability to understand surfaces and complex materials (such as alloys) and on that basis control their properties is a top priority in future research. Corrosion studies will benefit from further advances in surface characterisation and *in situ* methodological development.

Future potential of the area

Understanding corrosion mechanisms and developing measures to mitigate corrosion-induced breakdown will remain a high priority for applied research. Future advances in this field of major importance to society are likely to depend on improved fundamental understanding and the use of state-of-the-art characterisation methods, preferably in operating conditions.

Overall assessment

Svensson has a sound and fundamental approach to key issues in high-temperature steel corrosion. The research involves investigation of chromia vaporisation and its effects on the corrosion behaviour of iron-chromium alloys. It constitutes a unique effort that includes Corrosion Chemistry, Solid State Chemistry, Microscopy and Theoretical Chemistry. The research is rated as *very good* to *excellent* by the expert panel, and future funding is *strongly recommended*.

Zoltán Szabó

Division of Inorganic Chemistry, Department of Chemistry,
Royal Institute of Technology

Photochemical reactions of the uranyl ion

Summary of the research programme

The ligand-substitution chemistry of the trans-dioxo uranyl ion has been investigated with an arsenal of NMR techniques. The implications of ligand-exchange chemistry have been considered in the context of the uranyl ion's interaction with nucleotides. In addition, the photoinduced, hydrogen-atom abstraction photochemistry of the uranyl ion with hydroxycarboxylic acids, amino acids, oligopeptides and other biomolecules has also been examined.

Past performance

Methodology

Complex formation and ligand-exchange dynamics of the uranyl ion have been examined by means of 1D inversion transfer and 2D exchange spectroscopy, line-shape analysis and other 1D and 2D magnetisation-transfer experiments.

Position in the area

The research performed is of high quality and Zoltán Szabó's results have attracted attention from members of the actinide chemistry community. The research might have a higher profile with a more judicious choice of target. The uranyl ion has little practical use as a reagent in Chemistry or Biology.

Particular achievements

Despite the reactivity of the uranyl ion to small molecule substrates, uranium(VI)–nucleotide systems do not promote internucleotide bond formation. Szabó has made intelligent use of incorporated fluoride in the parent $UO_2(H_2O)_5$ complex to make the exchange kinetics of the ion amenable to studies with ^{19}F NMR. He has shown that phosphate and hydroxyl groups of the sugar bind the ion and deactivate it at a high pH.

Future prospects

Project plans

Szabó intends to examine the reaction of actinides more exotic than uranium with biomolecules at the forthcoming European NMR 'hot lab'. He will be stepping down from his current position and taking up a position as Senior Lecturer in Organic Chemistry at the Royal Institute of Technology in Stockholm.

Balance between resources and goal

The project has no student or postdoctoral research associates. Szabó has connections with *Institut für Nukleare Entsorgungstechnik* in Karlsruhe and the EXAFS beamline in Grenoble. Both of these facilities are of great benefit to Szabó's research in the area of actinide chemistry.

Comments on the area

Position in Inorganic Chemistry

With NMR used as an analytical tool, high-throughput screening procedures have been developed to examine ligand substitution. Careful multinuclear NMR studies have corrected previous errors in the literature. These are notable contributions to the field.

Importance of the area

The area of metal–nucleotide interactions and the interactions of metals with biomolecules is central in Bioinorganic Chemistry. As an indication of the importance of the area, there are entire Gordon Research Conferences on these subjects.

Future potential of the area

The interaction of metal complexes with nucleotides is an important area of research that may, in some cases, lead to new cancer therapies. Consider, for instance, the rich history of cisplatin and its derivatives. However, it is difficult to see how uranyl will ever be useful in this regard. Moreover, the photochemistry of uranyl is less compelling than of other photoreagents.

Overall assessment

Szabó specialises in NMR methodologies and has used this expertise to examine metal–oligonucleotide interactions. For his future research efforts, Szabó will benefit from developing a scientific vision by targeting an important problem of interest to the community at large.

The expert panel rates the research of Szabó as *good* to *very good* and *recommends* continued funding.

Reine Wallenberg

Division of Polymer and Materials Chemistry, Department of Chemistry, Center for Chemistry and Chemical Engineering, Lund University

Nanostructured functional materials

Summary of the research programme

This research project comprises three parts: 1) research connected to solid-oxide fuel cells, in particular the electrode materials; 2) structures of semiconducting nanowires in one, two and three dimensions, and the possible combination of elements in these wires; and 3) electron microscopy techniques applied to 'soft' materials in, for example, biological systems.

In the first subproject, new synthesis methods are being developed for strontium titanate as the basic structure for a conducting, porous electrode material. Glycine-nitrate combustion synthesis, yielding a mesoporous material consisting of nanometre-sized particles, is employed. These materials are characterised by several methods, such as BET, impedance spectroscopy, PXRD, XANES, HREM, SEM and XEDS. The effects of Sr/Ti-ratio and dope $SrTiO_3$ are probed with Nb during synthesis, and this has shown promising results.

In the second subproject, new electronic components on a true nanoscale are being developed, using MOCVD and similar techniques. Nanowires are made by a catalytic seed particle, and this can also be applied to growth of side branches, forming 'nanotrees'. These nanotrees can be made to interconnect and, in turn, form 3D devices. These structures and devices are strictly confined by the crystallography, the strain between epitaxial segments and the chemical composition, and it is essential to characterise the formed crystal structures at the atomic level, to understand and improve their behaviour. Recently, it has been shown that Si and III-V elements can be combined in a single nanowire, finally joining the worlds of Silicon Technology and Optronics.

Subproject 3) deals with materials on the borderline between bioorganic and inorganic materials, such as bone-replacement cement and unwanted precipitates in supersaturated body fluids, and is developing techniques for investigation of these systems.

Past performance

Methodology

This project, funded by the Swedish Research Council, focuses on solving solid-state crystallographic and structural problems on the nanometre level by means of local analytical techniques. Special attention is devoted to developing and implementing techniques to enhance information from High-Resolution Transmission Electron Microscopy (HRTEM). Operating cryo-HRTEM in this way has shown atomic resolution for nanoparticles in solution.

Position in the area

Reine Wallenberg's group has a strong reputation and is well known and well cited in the field. Even when the well-recognised joint publications with the Lund physicists (Professor Lars Samuelsson *et al*.) are excluded, Wallenberg is very well cited for his research accomplishments. Extended collaborations with several Swedish (the Nanometer Structure Consortium in Lund) and international scientists illustrate the group's strong position.

Particular achievements

The first publication of ordered arrays of epitaxial nanotrees and the formation of 3D networks of interconnected nanotrees should be mentioned as important and genuine highlights.

Future prospects

Project plans

The plans for the future clearly show that there will be sufficient knowledge and expertise and also innovation to compete internationally in the areas of Materials Chemistry and Structural Chemistry. Wallenberg will continue to spend time as a coordinator of the nanostructural consortium.

Balance between resources and goal

Excellent equipment and technical infrastructure for performing research at a high level appear to be present. For equipment replacement, money from the Swedish Research Council should be available regularly. Continuous support from the Research Council for PhD students and postdoctoral researchers, enabling Wallenberg to undertake new activities, is essential.

Comments on the area

Position in Inorganic Chemistry

Wallenberg has obtained a highly influential and well-recognised position as scientist and as coordinator of the nanostructural consortium, further enhanced by his close interaction with local physicists.

Importance of the area

Nanoscience and structural research with HREM and related techniques have a major bearing not only on advanced research, but also on highly skilled technical services, such as scanning electron microscopy, for other labs.

Future potential of the area

This research area is likely to remain very strong for several years.

Overall assessment

Wallenberg is supervising and inspiring an important and impressive project, applying several EM techniques to inorganic materials. His collaboration with physicists has proved crucial and successful. The Chemistry contribution alone is already at a very high level. Wallenberg's research is rated as *excellent* to *outstanding* by the expert panel. Continued funding is *most strongly recommended*.

Ola Wendt

Division of Organic Chemistry, Department of Chemistry,
Center for Chemistry and Chemical Engineering, Lund University

Organotransition Metal Chemistry: activation of small molecules

Summary of the research programme

The common theme of Ola Wendt's research is activation of small molecules and unreactive bonds. This project focuses on development of new organotransition metals, primarily in the area of 'green' Reaction Chemistry, with the aim of creating new starting materials for the chemical industry from such underutilised carbon sources as carbon dioxide and certain hydrocarbons. Kinetic and structure–reactivity relationships are sought in order to provide the requisite mechanistic detail to guide future targets of opportunity. One study involves the investigation of carbon dioxide reactions of M–O and M–C bonds with the goal of performing catalytic carboxylation of hydrocarbons and alcohols to carboxylic acids and organic carbonates. For this work, metal pincer and early metal metallocene complexes have been targeted. Another effort makes use of gold complexes for C–H activation for incorporation into well-known catalytic systems such as cross-coupling reactions.

Past performance

Methodology

The methods used in this project are synthesis, including specialised high-vacuum techniques and characterisation by multi-nuclear NMR and X-ray diffraction. There is sufficient expertise in the Wendt group to carry out their own solution and solid-state structure determination. Reactions are monitored by NMR spectroscopy to obtain kinetic information and theoretical calculations are being conducted in order to understand the observed reactivity patterns.

The project is collaborative, with a long-standing interaction with Professor Andreas Roodt, University of the Free State, Bloemfontein, South Africa, who is interested in mechanisms of fundamental organometallic reactions of the late transition metals. Six students have visited Wendt from South Africa to perform NMR measurements of exchange reactions and olefin metathesis and to carry out X-ray crystallography. Students from Lund

have spent time in South Africa performing synthesis and high-pressure IR measurements. Other collaborations are with Professor Henry Ssekalo of Makerere University, Kampala, Uganda (one joint student works on the catalytic applications of polyoxometallates); Professor Lars Öhrström, Chalmers University of Technology, Göteborg (collaboration on characterisation, use and description of coordination-compound-based 3D networks); Senior Lecturer Joachim Schnadt, Synchrotron Physics, Lund University (collaboration on synthesis and characterisation of solid-state materials for catalysis); and Senior Lecturer Kenneth Wärnmark, Organic Chemistry, Lund University (collaboration on supramolecular compounds based on transition metals, particularly their characterisation by means of synchrotron X-ray crystallography).

Position in the area

Wendt is a fine representative of a field that is very much underrepresented in Sweden. He is competitive in relation to other young researchers in the area but, given his relative lack of resources, cannot be expected to produce as much. This area should be supported in Sweden, where there are very few inorganic organometallic chemists, especially younger faculty members.

Particular achievements

In the chemistry of carbon dioxide, the pincer ligand phosphorus–carbon–phosphorus (PCP) framework has been used extensively in Pd and Pt chemistry. It was found that, although ordinary Pd-alkyl complexes are not reactive to carbon dioxide, methyl complexes with the PCP ligand have a very weak, highly reactive Pd-methyl carbon bond owing to the influence of the in-plane aryl group. X-ray crystallography has revealed it to be the longest Pd-methyl bond in a mononuclear complex known to date. The Pd-methyl bond reacts with carbon dioxide to form a new C–C bond. This result has been used in catalytic carboxylation of dimethyl zinc.

Complexes of the (PCP)PdX type (where X is a halide) were used as pre-catalysts for cross couplings and found to display very high thermal stability and activity, with the highest turnover rates reported to date. A subsequent mechanistic investigation of these processes revealed that it is severely inhibited by elemental mercury. This has led to the conclusion that the Pd pre-catalyst is reduced to Pd(0). This means that the catalysis involves the usual Pd(0)-Pd(II) cycle. Suzuki coupling studies have indicated that the Pd ion remains in a higher oxidation state.

Future prospects

Project plans

Further work on the chemistry of carbon dioxide will be carried out, with studies of the reaction mechanism of Pd–C and Zr–O insertions. Wendt also plans to look for more reactive Pd compounds for carboxylation of less reactive nucleophiles, with companion studies of platinum model systems. His work on polyoxometalate-supported catalysts will continue, with a focus on the gold catalyst used by Wendt for oxidation reactions. New work will include oxidation of arenes and alkanes.

Direct C–H activation using gold will also be attempted. The plan is to use well-defined gold catalysts for activation of arenes and try to connect this with well-known Pd Chemistry for biphenyl synthesis (Au(I) transfers aryl groups to palladium). Wendt has obtained preliminary results that support the conclusion that the reaction works.

To pursue all these lines of investigation successfully, Wendt will need a larger group and additional funding. As far as equipment is concerned, he appears to be well placed.

Balance between resources and goal

Wendt is a talented organometallic chemist who has managed to secure sufficient funds to be 100% active in research if he so wishes. In the period 2003–07, he has supervised three PhD students (and cosupervised a fourth) and 20 undergraduates, and published 26 articles. He has used his grant money very effectively and has the equipment he needs to carry out synthesis as well as characterisation experiments (X-ray, NMR). Continued funding is therefore recommended.

Comments on the area

Position in Inorganic Chemistry

Organometallic Chemistry is a central part of modern Inorganic Chemistry and there is every reason to believe that it will continue to flourish, especially in terms of 'green' Chemistry and catalysis, which are one focus of Wendt's project.

Importance of the area

Pincer Ligand Chemistry as applied to homogeneous catalysis is a very 'hot' topic in the field of Inorganic Chemistry, and one that continues to grow. In the US, more and more young people are joining the ranks and designing new phosphorus–nitrogen–phosphorus (PNP) ligands.

Future potential of the area

The potential for growth is, as already noted, very high. The expert panel predicts that, with the pincer-ligand platform, numerous new catalytic processes will be discovered and these will pave the way for future developments.

Overall assessment

International exposure of Wendt is recommended and he should be urged to go on a sabbatical where he can gain more theoretical knowledge of the area of mechanistic modelling, so that he can bring it back with him. Wendt's research is rated *excellent* and continued funding is *most strongly recommended*.

Gunnar Westin

Department of Materials Chemistry, Uppsala University

Solution chemical processing of complex nanomaterials, from molecules to materials

Summary of the research programme

The project is about understanding and controlling every step in the formation of solution-based materials. One focus is on the formation of complex materials, from precursor molecules and clusters to materials, by tailoring compounds containing homogeneous or heterogeneous clusters and eventually forming doped and core-shell structures, or thin polycrystalline or epitaxial films, which are currently of high interest for many application areas. Two such classes of materials have been chosen as targets: large-band-gap semiconductors and perovskites.

Specific subgoals of the project have been:

- To synthesise and characterise alkoxide molecules of 3d- and/or 4f-elements in detail and obtain further understanding of their formation, size, shape and heterometallic composition.
- To use these molecules in the synthesis of complex materials of high current interest and study the process stages from precursor to gel or nanoparticles and the final material in detail.
- To find a route for preparing controlled size clusters, inclusions and homogeneous dopings in a large-band-gap semiconductor, oxide thin film or nanoparticles (for diluted magnetic semiconductors).
- To find various routes to complex nanostructured porous materials based on large-band-gap semiconductors for photocatalytic decomposition of water to H_2 and organic groups to CO_2.
- To find routes to high-quality perovskites, such as polycrystalline, and epitaxial thin films.
- To understand the structure–property relationship, thereby helping to refine the new materials.

Past performance

Methodology

Gunnar Westin started this project by using Solution Chemistry to prepare material clusters based on alkoxides. He uses a wide range of techniques and

methods in addition to advanced synthesis. To characterise the products a broad array of experimental techniques has been used, the most important ones being thermal analysis, X-ray diffraction (powder, films, single crystals), IR, Raman, UV-Vis-NIR spectroscopy, SEM-EDS and TEM-ED-EDS. He also, in collaboration with experts elsewhere, uses many other techniques, such as XPS, synchrotron-based EXAFS, wide angle X-ray scattering, electric and piezo-electric measurements and magnetic susceptibility studies.

Position in the area

Westin has been quite productive since his PhD, which was obtained at a fairly advanced age; his list of publications shows high productivity; and many of them are already well cited, although his PhD was defended just over 12 years ago. Several invitations to speak at meetings have been received and he is an Editorial Board member of the *International Journal of Nanotechnology*.

Particular achievements

Westin's research on metal alkoxides, started only in the mid-1990s, has already led to many good publications in high-ranking journals. His work has also already culminated in six patent applications.

Future prospects

Project plans

The plans to undertake new research, as described by Westin in his oral presentation, appear vibrant and challenging. Uncertainty about the future of funding in Sweden, as sensed by the expert panel, might prompt advising Westin to spend some time abroad to gain even more recognition.

Balance between resources and goal

Given the researcher's past performance and ambitious plans, continued funding — and on a higher level than to date — is highly recommended.

Comments on the area

Position in Inorganic Chemistry

The chemistry of metal alkoxides as material precursors is challenging and still full of possibilities that will lead to totally new materials, like polycrystalline or epitaxial films. Westin has developed a prominent position in this area.

Importance of the area

The area of Solution Inorganic Chemistry is important and relevant to study and as a field, it should be maintained in the inorganic community of Sweden and if possible even strengthened.

Future potential of the area

This area of research, inspired by material precursors, will remain very important worldwide and should be studied by some few groups in Sweden as well.

Overall assessment

Westin has made important contributions since his 1995 PhD in the field of Molecular and Solution Coordination Chemistry. His work has attracted significant interest from others in and outside Sweden, most recently resulting in a transfer from Stockholm University to Uppsala University. The quality of the research is rated *very good* by the panel and continued funding, if possible on a larger scale than to date, is *strongly recommended*.

Xiaodong Zou

Department of Physical, Inorganic and Structural Chemistry, Stockholm University

Design of functional porous materials

Summary of the research programme

This project focuses on design, synthesis and characterisation of new functional microporous crystalline materials with special pore structures. These pore structures include large and extra-large micropores, intersecting channel systems and chiral or helical channel systems. Inorganic, metal-organic and organic molecules are used as blocks to build open framework structures whose properties will reflect their chemistry, pore sizes and shapes. The main objectives are to synthesise porous materials from molecular building units and/or clusters; to study the crystal chemistry of these materials; and to develop crystallographic methods for studying porous and other complex structures. As materials, zeolites and related porous compounds find vast applications in catalysis, adsorption, separation, ion-exchange, nanosensors and host–guest assembly. One key objective of the project is to develop new functional crystalline open-framework materials, especially germanates and germanate-related materials. The open-framework germanates are synthesised mainly through hydrothermal and/or solvothermal synthesis, with organic amines used as structure-directing agents. The ultimate goal is to advance synthesis of open-framework materials towards rational design. The materials are characterised with a variety of methods. Electron microscopy and crystallography are key methods of studying the structures of nanosized crystals at their initial crystallisation stage. The interrelationships of properties, structure and synthesis are another topic of study.

Past performance

Methodology

Xiaodong Zou uses template-based solvothermal synthesis as a route towards novel micro- and mesoporous materials. She has very successfully developed a large number of novel germanium-based materials, including two new types of zeolite framework topologies. Other materials represent analogues to MCM-type mesoporous structures. Electron microscopy is a key tool for the structural analyses. Zou has made significant contributions to the development of electron crystallography as a tool for analysis of complex structures and microporous materials.

Position in the area

Zou has an internationally leading position in Electron Crystallography and is well recognised for her excellent work on novel micro- and mesoporous materials.

Particular achievements

With respect to Inorganic Chemistry and materials, Zou's achievements regarding synthesis and structure determination of novel micro- and mesoporous germanates are important. These contain variously shaped and composed building entities ('clusters') and include crystalline analogues to mesoporous MCM-48 and -41 with large-sized pores. In electron microscopy, Zou has developed a method for 3D reconstruction of TEM patterns and applied it to zeolite-beta polymorph B, for example.

Future prospects

Project plans

Zou's future plans indicate several directions: structure determination by Electron Microscopy methods; synthesis of novel micro- and mesoporous germanates; studies to enhance understanding of growth mechanisms for solvothermal synthesis of germanates; and expansion into the area of metal-organic framework structures. The latter includes functionalisation and applications in catalysis, although their utility may be limited by their physical and chemical instability.

Balance between resources and goal

Zou is well placed at Stockholm University and appears to have ample funding from various sources, including a Berzelii Centre. Overall, the funding provides a good balance between the highly ambitious goals and the resources available.

Comments on the area

Position in Inorganic Chemistry

Solvothermal synthesis is a central synthetic tool in Inorganic Chemistry used for making microporous materials. Development of such routes towards micro- and mesoporous germanates represent significant advances in this respect and expands our understanding of Inorganic Structure and Materials Chemistry. Electron Crystallography and its development represent an important method of elucidating complex inorganic structures, particularly in cases where X-ray diffraction is not feasible owing to a lack of appropriate crystals.

Importance of the area

Development of novel microporous materials is of general interest for expanding knowledge of inorganic materials and structure types. Many such compounds may also find applications, given sufficient chemical and thermal stability. Electron Diffraction (and Crystallography) is a key area, and will become even more important in the future for analysing complex or nanostructured materials on different length scales.

Future potential of the area

The area of micro- and mesoporous materials has major potential for applications, in particular when the compounds are chemically modified by means of functionalisation. Such tools as electron microscopy are, and will continue to be, most important for analysing complex or nanostructured materials on various length scales.

Overall assessment

Zou's work on novel microporous and mesoporous germanates, as well as the development of Electron Crystallography for structure analysis and its application to porous crystalline materials, is of very high quality. These fields are considered to be of high importance for the future. The expert panel rates the research as *excellent*. Further funding is *most strongly recommended*.

Lars Öhrström

Physical Chemistry, Division of Chemistry and Biochemistry, Department of Chemical and Biological Engineering, Chalmers University of Technology

Crystal Engineering of 2D and 3D networks — synthesis, analysis and applications

Summary of the research programme

Crystal engineered networks, including metal-organic frameworks (MOFs), are under investigation with the goal of developing new solids for applications as porous materials for chiral catalysis and separation, nonlinear optics, magnetic materials and hydrogen storage materials. The work is aimed at an understanding of the intermolecular interactions that control the self assembly of molecular-based 3D frameworks.

Past performance

Methodology

The key experimental method employed for this project is single crystal X-ray diffraction. Lars Öhrström's background in Synthetic Organic and Inorganic Chemistry greatly enhances the potential of this research effort.

Position in the area

Öhrström is preparing some interesting solid-state supramolecular compounds. The supramolecular work has garnered the community's attention and this work has been relatively well received.

Particular achievements

Öhrström has singled out four related areas of science, all connected with the assembly of molecules in 2D and 3D nets in the solid state:

(1) Öhrström is attempting to understand the interactions that control 2D and 3D networks. Working with Dr. Ola Wendt, he has sought to understand the assembly of Pd pincer compounds in the solid state. Owing to hydrogen bonds between the tetragonal complexes, chiral channels form from the solid-state packing of these molecules.

(2) 2D and 3D nets are being analysed with a 'structural network approach'. A database of key structure elements is being constructed, with the goal of building structures from the bottom up.

(3) With insights provided by the structural network approach, Öhrström is attempting to design solids on an a priori basis. The work has led to the preparation of interesting 3D structures derived from tris-chelated octahedral complexes with bis-bidentate ligands. Using this approach, a series of porous metal-organic frameworks (MOFs) of composition $M[Co(ox)_2(en)]_{2.x}H_2O$, some of them chiral, have been prepared.

(4) Öhrström and his students have built interpenetrating 2D square networks, overlaid with a secondary square network.

Future prospects

Project plans

Öhrström will continue to explore the multicomponent coordination polymers. Several intriguing questions, one being how a single component (such as the inclusion molecule) affects the intermolecular interactions of the multicomponent array, remain.

Balance between resources and goal

The project involves small staff inputs from two PhD students. The work depends heavily on X-ray crystallography, but the group lacks direct access to any instrument. Considering the central emphasis on Structural Chemistry in this research project, the absence of open access to instruments severely hinders its productivity. The project would benefit from an organisational structure that allowed unimpeded access to the single-crystal X-ray instrument at Chalmers University of Technology and Göteborg University. An increase in the current grant size for this purpose may be necessary.

Comments on the area

Position in Inorganic Chemistry

Öhrström is examining crystal-engineered materials based on hydrogen bonding and metal-organic frameworks. With regard to the former, Öhrström may revisit many of the same problems that plagued Crystal Engineering in the 1980s and early 1990s. Energetics other than hydrogen bonds can overwhelm the hydrogen bond. The MOF approach holds promise,

given that the solids are built from metal–ligand bonds. With his book on molecule-based materials, Öhrström has also contributed to popularising science through popular education.

Importance of the area

Porous 'designer solids' have a variegated array of applications, including separations, hydrogen storage and other gas storage. To achieve predictability in designing such solids from a rule set would represent a significant advance.

Future potential of the area

Several years ago, Crystal Engineering was at the forefront of Chemistry. After nearly a decade of work, interest in this area subsided owing to the difficulty of controlling the subtle energetics of molecular interactions underlying crystal lattice formation. Very few structures were designed *a priori*. Subsequently, however, it proved feasible to rationalise many, using Crystal Engineering concepts. Renewed interest in the area has been boosted by the development of metal-organic frameworks. These structures are based on robust metal-organic bonds. Accordingly, solids can now be built from these materials with some predictability.

Overall assessment

Öhrström is preparing some very interesting supramolecular solids. The expert panel believes that, in the long run, Öhrström's research will benefit from a demonstration of some type of function (such as magnetism) of designed solids emanating from this research. The research is rated as *very good* by the panel and continued funding is *strongly recommended*.

ACKNOWLEDGEMENTS

On behalf of the Swedish Research Council, we would like to express our sincere gratitude to the members of the international expert panel. The work involved was considerable, and its successful completion would not have been feasible without the members' collective expertise, integrity and vigorous, dedicated efforts. Evaluating and assessing the work of peers is invariably a highly demanding task. Moreover, doing so in the very broad and diversified area of Inorganic Chemistry requires great proficiency and expertise.

The present panel has consistently met these requirements and we have been most impressed by the professionalism its members have shown. They have conducted all the interviews in a congenial and non-stressful manner while retaining a focus on the key issues. They have also succeeded in obtaining information not only about the individual projects but also concerning the structural problems involved.

We also wish to thank the scientists under review for the time and trouble they have taken to compile the requisite material on their research projects, which has been an indispensable reference base for the evaluation process.

Finally, we would like to express our gratitude for the assistance that has been provided by staff members at the Swedish Research Council.

Bo Albinsson
Rapporteur

Winnie Birberg
Secretary

APPENDIX 1

Background of the experts

Professor Kim Dunbar

Department of Chemistry, Texas A&M University, United States
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- *Born* in Mount Pleasant, Pennsylvania, USA;
- B.S. (Chemistry) 1980;
- Ph.D. (Inorganic Chemistry) 1984;
- Postdoctoral Research Associate, 1985–1986.

Employment History

Research and Teaching Assistant, Purdue University, 1980–1984; Postdoctoral Research Fellow, Texas A&M University, 1985–1986; Assistant Professor, Michigan State University, 1987–1990; Associate Professor, Michigan State University, 1991–1992; Professor, Michigan State University, 1993; University Distinguished Professor, Michigan State University, 1998–1999; Professor, Texas A&M University, 1999; Davidson Professor of Science Chair, Texas A&M University, 2004; Distinguished Professor of Chemistry, Texas A&M University, 2007.

Special Assignments

Panelist, NSF Postdoctoral Research Fellowships in Chemistry, 1991; Camille and Henry Dreyfus Teacher-Scholar Award, 1991–1995; Fellow, the Alfred P. Sloan Foundation (1992–1995); Councilor, ACS Division of *Inorganic Chemistry*, 1995–1997; Panelist, ACS Scholars Program, 1996–1998; Minority Affairs Committee, 1996–2000; Advisory Board, Accounts of Chemical Research, 1997–1998; Advisory Board, Inorganic Chemistry, 1997–1998; Sigma Xi Research Award, Michigan State University, 1998; Plenary Lecturer, XXXIII ICCC Conference, Florence, Italy, 1998; Distinguished Faculty Award, Michigan State University, 1998; Vice-Chair, Inorganic Gordon Conference , 1998; Advisory Board, Inorganic Chemistry Communications, 1998–2003; CHEMTRACTS, 1998–present; Chair, Inorganic Gordon Conference, 1999; Member of the Council, Gordon Research Conferences,

1999–present; North American Advisory Board, *Journal of the Chemical Society Dalton Transactions*, 1999–present; Distinguished Alumni Award, Westminster College, 2000; NSF Advisory Board on Research Misconduct in Biochemistry, Chemistry and Microbiology, 2000–2002; Advisory Board, *Crystal Engineering*, Advisory Board, *European Journal of Inorganic Chemistry*, 2000–present; Sigma Xi Chemical Honorary; NASA Sharp Plus Mentor, 2001; NSF Creativity Award, 2002; Secretary, ACS Division of Inorganic Chemistry, 2002–2004; Associate Editor, *Inorganic Chemistry*, 2002–present; Fellow, American Institute of Chemists, 2004; Fellow, American Association for the Advancement of Science, 2004;.Elected Fellow, American Association for the Advancement of Science, 2004; Purdue University Department of Chemistry Distinguished Alumna Award, 2004; American Advisor for MolMAGNet, the European Funding Network on Research in Magnetism, 2005–2008; Chair, Texas A&M Section of the American Chemical Society, 2006; Chair, ACS Texas A&M Local Section, 2006; The Association of Former Students Distinguished Achievement Award for Graduate Mentoring, 2006; American Chemical Society Chair, ACS Division of Inorganic Chemistry, 2007.

Scientific Activities and Interests

Topics in synthetic, Structural and Physical Inorganic and Bioinorganic Chemistry; the use of a range of tools including spectroscopy, X-ray crystallography, magnetometry, electron microscopy, mass spectrometry and electrochemistry reflect the breadth of problems under investigation.

Professor Helmer Fjellvåg

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- *Born* in Norway in 1954;
- Cand. Real. (Chemistry) University of Oslo 1978.

Employment history

Research Scientist; University of Oslo and Institute for Energy technology, Kjeller, Norway, 1978–1983 and 1985–86; Research scientist, Max Planck Institut für Festkörperforschung, Stuttgart, Germany and Institut Laue Langevin, Grenoble, France, 1984–1985; Associate Professor, University of

Oslo, 1987–1991; Adjunct professor, Physics Department, Institute for Energy Technology, Kjeller, 1991–present; Professor, Department of Chemistry, University of Oslo, 1992–present; Sabbatical leave, European Synchrotron Radiation Facility and ILL, Grenoble, 1996; Sabbatical leave, Visiting Professor, Tokyo Institute of Technology, 2003; Director, Centre for Materials Science and Nanotechnology, University of Oslo, 2003–present; Core member of the *inGAP* centre for researched based innovation, 2006–present.

Special Assignments

Member, ESRF Review committee, 1994–1996; Board member, Swiss Norwegian Beam Line, ESRF, 1995–2000; Member, the Norwegian Academy of Science and Letters; Awarded the Birkeland innovation prize, 2006; ESRF Council member, 2007–present; Board member, Nordsync, 2007–present.

Scientific Activities and Interests

Inorganic chemistry and materials science: synthesis – characterization – theory /modeling: inorganic synthesis, materials chemistry, thin films – sol-gel, ALCVD, nanoparticles and multilayered films, solar cell materials, complex oxides, powder X-ray and neutron diffraction, magnetic and multiferroic materials, microporous materials for adsorption and catalysis, intermetallics and hydrogen storage, battery materials, electronic structure, stability. Published around 320 publications in international journals with referee. Holds several patents and is co-founder of a spin-off company (coatings).

Emeritus Professor Erik Larsen

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- *Born* in Denmark in 1937;
- Mag. Scient. (Chemistry) Copenhagen University 1961;
- Doc. Scient. (Coordination Chemistry) Copenhagen University 1980.

Employment History

Amanuensis at Chemistry Laboratorium I, University of Copenhagen, 1961–1964; Lecturer, University of Copenhagen, 1964–1980; Visiting lecturer at University of East Anglia, England, 1965; Research Associate (Nato) at Massa-

chusetts Institute of Technology, USA, 1970–1971; Full Professor, Chemistry Department, The Royal Veterinary and Agricultural University, 1980–2007; Emeritus Professor, University of Copenhagen, 2007–present.

Special Assignments

Member of Danish Natural Sciences Research Council, SNF, 1993–1999; Chairman SNF, 1995–1999; Member of PESC, Subcommittee for Physical and Engineering Sciences, of European Science Foundation, 1995–2001; Member of the PESC Core group, 1998–2001; Member of CERC3, 1994–2001; Chairman CERC3, 1999–2000.

Scientific Activities and Interests

Coordination chemistry; Synthesis; Thermodynamics of coordination compounds; the carbonanion-cobalt(III) bond; Spectroscopy; Chirality; Circular dichroism measured and computed; Ligand field theory; Density functional computations; History of chemistry and science's influence on history. Published ca 100 peer-reviewed research publications, three books, contributed to two books on historical aspects and some publications in Danish.

Professor Daniel G. Nocera

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- *Born* in USA in 1957;
- BS (Chemistry) Rutgers University 1979;
- Ph.D. (Chemistry) California Institute of Technology 1984.

Employment History

Assistant Professor of Chemistry, Michigan State University, 1983–1988; Associate Professor of Chemistry, Michigan State University, 1988–1990; Professor of Chemistry, Michigan State University, 1990–1997; Associate Director, Center for Fundamentals Materials Research, Michigan State University, 1993–1996; University Distinguished Professor, Michigan State University, 1997; Professor of Chemistry, Massachusetts Institute of Technology, 1997–present; W. M. Keck Professor of Energy, Massachusetts

Institute of Technology, 2002–2007; Faculty Member, Earth Systems Initiative, MIT, 2003–present; Henry Dreyfus Professor of Energy, Massachusetts Institute of Technology, 2007–present.

Special Assignments

Alfred P. Sloan Fellow, 1990; National Research Council Outstanding Young Investigator, 1991; College of Natural Science Distinguished Faculty Award, Michigan State University, 1996; University Distinguished Faculty Award, Michigan State University, 1997; Scientific Advisory Boards: Polaroid Corporation, 1998–2001, IDP, 2002–2006; Eni Technologies, 2005–present; BioDesign Institute, 2005–present; Ceramatec, 2008-present; Metallobiochemistry Study Section, National Institutes of Health, 1998–2002; Editor, *Inorganic Chemistry Communications*, 1998–2002; Chair, Editorial Board, *ChemSusChem*, 2007–present; Board of Editors: *Inorganic Chemistry*, 1994–1996 and 2004–2006; *Accounts of Chemical Research* 2001–2003; *Journal of the American Chemical Society* 2005–present; *Comments in Inorganic Chemistry*, 2004–2006; *OIL*, 2007-present; Eni-Italgas Prize for Energy and the Environment, 2004; American Academy of Arts and Sciences, 2005; MIT School of Science Prize for Excellence in Undergraduate Teaching, 2005; President's Energy Research Council, MIT, 2005–2006; Panel Chair, DOE Basic Research Needs for Solar Energy in 2005, Catalysis in 2007, and Electric Energy Storage in 2007; Member, NSF and NIST Workshop on Enhancing Innovation and Competitiveness Through Investments in Fundamental Research, 2006; I-APS Award in Photochemistry, 2006; DOE Basic Energy Chemical Sciences Council, Grand Challenges, 2006–2007; Inaugural Chair, Gordon Research Conference on Renewable Energy, 2007; Fellow, American Association for the Advancement of Science, 2007; Burghausen Prize, 2007; Mack Award, The Ohio State University, 2007; Global Agenda Council on Alternative Energies, World Economic Forum, 2008-present; Founder, Sun Catalytix, 2008; DOE Council for Chemical and Biochemical Sciences, 2007-2011; ACS Harrison Howe Award, 2008; ACS Inorganic Chemistry Award, 2008.

Scientific Activities and Interests

Biology and Chemistry of energy conversion; proton-coupled electron transfer; artificial photosynthesis; spin frustration and quantum spin liquids; nanocrystal chemosensors; multielectron photochemistry; global energy analysis and policy. Published over 250 publications, given over 450 invited talks and 38 named lectureships.

Professor Jan Reedijk

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- *Born* in the Netherlands in 1943;
- BSc (Chemistry), Leiden University 1964;
- MSc (Chemistry), Leiden University 1966;
- Ph.D. (Chemistry), Leiden University 1968.

Employment History

Junior Lecturer/Lecturer, Leiden University, 1966–1972; Senior Lecturer in Inorganic and Physical Chemistry, Delft University of Technology, 1972–1979; Professor of Inorganic Chemistry, Leiden University, 1979–present; Director of the Leiden Institute of Chemistry, 1983–2005; Visiting Professor, Cambridge University (UK), 1993; Visiting Professor, University Louvain la Neuve (Belgium), 2002; Visiting Professor, Université Louis Pasteur, (Strasbourg, France), 2005–present.

Special Assignments

President (and -elect), the Royal Netherlands Chemical Society, 1991–1993; Awarded the Max Planck Research Award in Chemistry, 1992; Elected Member, the Royal Netherlands Academy of Sciences, 1996; Elected Member, Finnish Academy of Sciences, 1997; Elected Honorary Member, Royal Netherlands Chemical Society, 2003; Elected Member, the Academia Europaea, 2004.

Executive Secretary, the International Conference on Coordination Chemistry (ICCC), 1988–present; Present and former member of the editorial boards of over 15 major chemistry journals, including the (founding) co-editorship of the rapidly growing *European Journal of Inorganic Chemistry* (merger from several European Chemical Society Journals).

Scientific Activities and Interests

Coordination Chemistry of transition-metal ions; Bioinorganic Chemistry (active-site structure and mechanism; models; metal-DNA interactions); applications of Coordination Chemistry in catalysis, medicine, ion-exchange, Surface Chemistry; Extended (magnetic; electric) interactions in coordination compounds (dimers, clusters, chains); Molecular recognition and intermolecular interactions (catalysis; biomacromolecules). Published over 1 100 peer-reviewed research publications, co-edited three books. Supervised over 200 MSc students, and over 150 PhD students and postdocs.

APPENDIX 2

Evaluation of Research Projects Supported by the Swedish Research Council

Inorganic Chemistry

1. Introduction

The Swedish Research Council is a government agency, headed by a Director General and Board, under the Ministry of Education and Research. There are some 140 employees. The Research Council contains three Scientific Councils, for Humanities and Social Sciences; Medicine; and Natural and Engineering Sciences. It also has a Committee for Educational Sciences and a Committee for Research Infrastructures.

A Secretary General is in charge of each subject group represented by the above-mentioned five Scientific Councils and Committees. The Secretary Generals, employed part-time for up to six years, are assisted by coordinators and heads of departments. The Scientific Councils and the Committees for Educational Sciences and Research Infrastructures are expert bodies that promote and support research of top scientific quality in their respective areas. They also assess ongoing research, evaluating its quality and importance, and monitor trends in Swedish and international research.

A majority of Board and Scientific Council members are appointed by an electoral committee that is, in turn, elected by researchers and teachers at higher education institutions (HEIs). The Swedish Government appoints the Chair and several members of the Board and Scientific Councils alike. The term of office for members, both elected and appointed, is three years. Members can serve a maximum of two consecutive terms.

The Board is responsible for overall strategy and policy. One of its responsibilities is to determine the Research Council's focus within the framework of goals and guidelines established by the Riksdag (Swedish Parliament) and Government. The Board also approves the organisation's overall work programme and settles issues of principle and strategy associated with activities to promote research.

In accordance with its Statutes, as laid down by the Government, the Swedish Research Council evaluates the research it supports financially.

For each scientific field, an expert panel is entrusted with this task. None of the experts are in any way involved in the projects under review. The panel is composed of scientists from outside Sweden, capable of assessing research projects in an international perspective and free from the influence of national considerations. Panel composition is based on proposals from the grantees undergoing evaluation. The Research Council attaches considerable weight to the advice given by these foreign experts and is most grateful for the positive response to its invitations to serve on the Council's expert panels.

The purpose of the evaluations is to inform the Research Council about the scientific quality of research projects in international terms. The projects are thus the principal objects of consideration. However, the expert panel is encouraged to comment on structural matters as well. Evaluations should be future-oriented where possible, and the panels' reports are key elements in the Council's future assignment of priorities.

The present document describes the evaluation process and the overall framework for its execution.

2. Work organisation and other procedural matters

The Scientific Council for Natural and Engineering Sciences appoints the Swedish Chair (who is also the rapporteur) of each international expert panel and also a research officer from the Swedish Research Council to serve as Secretary to the panel.

Each expert panel decides for itself on the distribution of work among its members. However, the Chair-cum-rapporteur and the Secretary propose a plan for allocating the tasks involved in compiling the report among the panel members. The final report is issued while the panel's work is still in progress, during its interviews with the grantees (compare points 3 and 4 below).

3. Collection and distribution of basic documentation

Each research project supported by the Swedish Research Council has a principal grantee responsible for the project. These grantees are requested by the Secretariat to submit scientific reports and other documentation on which the evaluation can be based. Points 3.1–3.8 below list what is normally requested. Details may, of course, vary depending on the subject and other factors.

3.1 A financial overview detailing the support granted by the Swedish Research Council over the past five financial years and support from other organisations in 2003–07.

3.2 A list of people involved in the project, including research and support staff, graduate students and visiting scientists, and a specification of overhead costs.
3.3 A summary of articles, papers and/or dissertations in the project over the past five years.
3.4 A brief account of current collaboration with other research groups in formal research projects, EU networks etc.
3.5 A summary of the research.
3.6 A brief account of the objectives and methods of the grant proposal submitted most recently.
3.7 A summary of the main results achieved in the project(s) evaluated.
3.8 Future plans.

4. Interviews

The written overviews serve as documentation for the interviews. Each interview is preceded by a short presentation by the grantee under review. A brief interview and discussion between the expert panel and the grantee follow. The panel convenes briefly after each interview to summarise and write a short report on the quality of the grantee's research.

5. Aspects covered in the evaluation

The documentation (point 3), the presentation and the interview (point 4) together form the basis of the evaluation. Points 5.1–5.7 below list the aspects or questions that the Research Council wishes to see addressed by panels in their reviews of individual projects. Experience of previous evaluations carried out by the Research Council has demonstrated the major benefits of this procedure. However, each panel is free to modify the procedure where it sees fit.

Aspects to cover are:

5.1 The scientific quality of the results obtained.
5.2 The scientific value of proposed projects (including any improvements that may be achieved by changing the aim and focus of the project).
5.3 The merits of the methods used and proposed.
5.4 The capability of the project leader and staff (including such issues as group size and composition).
5.5 The adequacy of existing and proposed research positions, facilities and equipment.
5.6 Other considerations or points of potential relevance to the projects.
5.7 Whether support should be increased, reduced or left unchanged, whether projects should be terminated and/or constructive alternative options, if any.

Specific questions may also be addressed to the expert panel by its principal, the Research Council. Such questions may relate to specific projects or to an entire scientific field.

6. Expert panel's report

The work of the expert panel culminates in a report to the Swedish Research Council. This report should contain a section containing comments on the overall scientific level, in an international perspective, of the research performed. The report should discuss any structural and organisational problems involved, and may raise any need for costly equipment and other points of general relevance. A further section should deal with the individual project in an international perspective, as outlined in point 5 above.

The expert panel should be aware that, owing to the constraints of the current budget situation, the Scientific Council for Natural and Engineering Sciences is obliged to reject some applications of excellent quality, and that many applications are necessarily funded at a suboptimal level.

To standardise the terminology used in assessment of individual projects, the following ratings should be used.

Outstanding (5)

Outstanding research in an international perspective, of great international interest, with a broad impact and with publications in internationally leading journals; the grantee is among the leading researchers, in an international perspective, in the whole field of research evaluated.

Excellent (4)

Research at a very high international level, of international interest, with an impact within its field and with publications in internationally leading journals; the grantee is among the leading researchers in Sweden in the field concerned.

Very good (3)

Research at a very good international level, with publications in internationally well-known journals; the grantee has a good international reputation in the field and the research should receive funding from the Swedish Research Council if possible.

Good (2)

Research of a good international standard, at least partially published in well-known international journals. To be rated as 'Good', the research should be of sufficient quality to qualify for funding from the Swedish Research Council, provided that funds are available for the purpose.

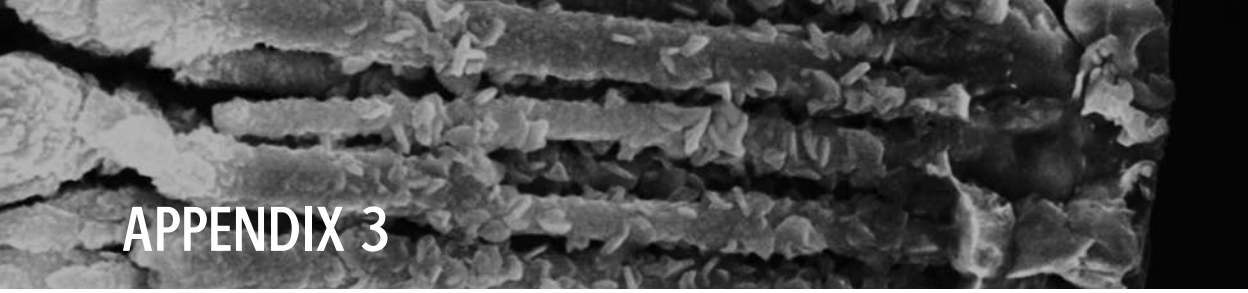
Insufficient (1)
Research of quality that is inadequate for funding from the Swedish Research Council. The rating 'Insufficient' does not necessarily mean that the research is of low quality. The research may be good but nonetheless of insufficiently high quality to meet the Research Council's stringent requirements.

The Research Council appreciates a discussion on action priorities in terms of both financial support and of structural issues.

To indicate the relative importance of different recommendations, the following expressions should be used: *recommends*, *strongly recommends* or *most strongly recommends*.

7. Handling and distribution of the report
The expert panel's report is presented to the Swedish Research Council and the Scientific Council for Natural and Engineering Sciences. It is also circulated to all grantees concerned and, on request, to universities and any other agencies or individuals who have expressed an interest in this kind of information. Under Swedish law, all reports of this kind are classified as public documents. Unsurprisingly, an evaluation report sometimes gives rise to comments by grantees whose work has been reviewed. If in writing, these comments are distributed to the members of the Scientific Council for Natural and Engineering Sciences.

8. Honorarium
Under the Swedish Research Council's regulations, a member of an expert panel receives a modest fee or honorarium. Members' travel costs and other expenses are defrayed or reimbursed by the Research Council.



APPENDIX 3

Abbreviations and Acronyms

AAS	Absolute Asymmetric Synthesis
AFM	Atomic Force Microscope
ALD	Atomic Layer Deposition
ALISTORE	Advanced Lithium Energy Storage Systems
ATR-FTIR	Attenuated Total Reflection Fourier Transform Infrared
BASF	Registered trademark
BET	Brunnaure–Emmett–Teller
CDC	Carbide-Derived Carbon
Chalmers	Chalmers University of Technology
Cryo-TEM	Cryogenic Transmission Electron Microscope
CVD	Chemical Vapour Deposition
DFT	Density Functional Theory
DMPU	N,N'-dimethylpropyleneurea
ECN	Energy Research Centre of the Netherlands
EM	Electron Microscopy
ESF	European Science Foundation
ESRF	European Synchrotron Radiation Facility
ESS	European Spallation Source
EXAFS	Extended X-Ray Absorption Fine Structure
FAP	Fluorapatite
FEG-TEM	Field-Emission Gun-Transmission Electron Microscopy
FIB	Focused Ion Beam
FT-IR	Fourier Transform Infrared Spectroscopy
FT-Raman	Fourier Transform-Raman
GDP	Gross Domestic Product
GPa	Gigapascal
GU	Göteborg University
HAP	Hydroxyapatite
HREM	High Resolution Electron Microscopy
HRTEM	High Resolution Transmission Electron Microscopy
HTC	Competence Center for High-Temperature Corrosion
ICT	Information and Communication Technology
IR	Infrared

ISIS	A pulsed neutron and muon source at the Rutherford Appleton Laboratory near Oxford, UK
KTH	Royal Institute of Technology
LAXS	Low-Angle X-ray Scattering
LCVD	Laser-assisted Chemical Vapor Deposition
LU	Lund University
MAX	A national Synchrotron Radiation Facility located in Lund, Sweden – operated jointly by the Swedish Research Council and Lund University
MAX	MAX-phase materials: three component materials with properties in between ceramics and metals
MCM	Part of the nomenclature of zeolite minerals
MFM	Magnetic Force Microscopy
MOCVD	Metal-Organic Chemical Vapour Deposition
MOF	Metal-Organic Framework
MRI	Magnetic Resonance Imaging
MSDC	Molecular Structure Design Concept
nCHREM	National Center for High Resolution Electron Microscopy
NMR	Nuclear Magnetic Resonance
OECD	Organisation for Economic Co-operation and Development
PCP	Phosphorus-Carbon-Phosphorus
PES	Photoelectron Spectroscopy
PI	Principal Investigator
PMG	Phosphono-methyl-glycine
PNP	Phosphorus-Nitrogen-Phosphorus
PXRD	Powder X-ray Diffraction
R&D	Research and Development
RMC	Reverse Monte Carlo
SEI	Solid Electrolyte Interface
SEM	Scanning Electron Microscope
SEM-EDS	Scanning Electron Microscope-Electron Detector System
SKPFM	Scanning Kelvin Probe Force Microscopy
SLU	Swedish University of Agricultural Sciences
SOFC	Solid Oxide Fuel Cell
SQUID	Superconducting Quantum Interference Device
SSF	Swedish Foundation for Strategic Research
SSRL	Stanford Synchrotron Radiation Laboratory
STINT	The Swedish Foundation for International Cooperation in Research and Higher Education

SU	Stockholm University
TEM	Transmission Electron Microscope
TEM-ED-EDS	Transmission Electron Microscope-Electron diffraction-Energy dispersive spectroscopy
UmU	Umeå University
UU	Uppsala University
UV-VIS-NIR	Ultra violet-Visible-Near infrared
VINNOVA	The Swedish Governmental Agency for Innovation Systems
XANES	X-ray Absorption Near Edge Structure
XAS	X-ray Absorption Spectroscopy
XEDS	X-Ray Energy Dispersive Spectroscopy
XMCD	X-ray Magnetic Circular Dichroism
XPS	X-ray Photoelectron Spectroscopy
XRD	X-Ray Diffraction

Support from the Swedish Research Council during the period of 2003–07*

Name	Type of funding	Reg. No.	Project title	2003	2004	2005	2006	2007	Total
Mats Boman	Project grant	2001-1587	Laser assisted synthesis and characterization of ultra-small size-selected nanoparticles from the gas phase and the liquid phase	520 000	520 000				
		2005-3308	Nanoporous alumina a versatile material in biochemistry to make a bioreactor, a nanopump and for chromatography				610 000	610 000	**2 260 000**
Yvonne Brandt Andersson	Project grant	2002-4211	Metal hydrides-syntheses, hydrogen absorbing properties, crystal structure and electronic band structure	561 080	561 080	561 080			
		2005-6101	Light metal hydrides-synthesis, characterisation and hydrogen absorbing properties of new magnesium alloys and compounds				607 500	607 500	
	Travel grant	2003-6389	Measurements at ISIS	35 200					
		2006-1100	Neutron diffraction measurements at the neutron source LLB, Saclay, Paris, France				24 200		
		2007-781	Neutron diffraction measurements at the neutron source LLB, Saclay, Paris, France					39 200	**2 996 840**
Jan-Otto Carlsson	Project grant	2001-2589	Chemistry at interfaces for materials design	845 000	845 000				
		2001-3156	Chemical processes for preparation of both thick and thin films of superconducting borides	780 000	780 000				
		2004-4738	Chemical processes at growth from the vapour; Aspects of mechanisms, film structure and properties			1 765 000	1 485 000	1 485 000	**7 985 000**

Name	Type of funding	Reg. No.	Project title	2003	2004	2005	2006	2007	Total
Kristina Edström	Project grant	2002-4109	Carbon Materials for Electrochemical Energy Storage	405 600	405 600	405 600			
		2003-4486	Nanostructured materials for energy storage		405 000	405 000			
		2005-3356	Nanostructured materials in electrochemical applications for energy conversion and storage				610 000	610 000	**3 246 800**
Sten Eriksson	Project grant	2002-5647	Synthesis, structure, dynamics and function; towards the design of complex oxides for materials applications	581 360	581 360	581 360			
		2006-3809	Synthesis of multifunctional magnetoelectrics by traditional and soft-chemistry routes: Guidance by DFT calculations, in-situ X-ray powder diffraction and TG/DTA					610 000	
	Travel grant	2003-1237	Measurements at ISIS, Rutherford Appleton Laboratory	23 800					
		2004-269	Measurements at ISIS, RAL, England		12 800				
		2004-7857	Measurements at ISIS, Rutherford Appleton Laboratory, England		25 700				
		2005-7681	Measurements at ILL, Grenoble			52 900			
		2005-8017	Measurements at ILL, Grenoble			13 800			
		2005-8482	Measurements at ISIS, Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire, England			41 000			
		2006-926	Measurements at ISIS, Rutherford Appleton Laboratory				19 200		
		2006-7435	Measurements at ILL, Grenoble				38 700		
	Equipment	2004-4465	4 K Cryocooler for neutron diffraction instruments			360 000			**2 941 980**

Name	Type of funding	Reg. No.	Project title	2003	2004	2005	2006	2007	Total
Saeid Esmaeilzadeh	Project grant	2001-1680	Nitrido-silicates	234 000					
		2003-2970	Nitrido-silicates		594 000	594 000			
		2005-3367	Functional nitrides and carbides of main group elements				610 000	610 000	**2 642 000**
Andreas Fischer	Project grant	2002-4416	Synthesis, structure, dynamics and function; towards the design of complex oxides for materials applications	270 400	270 400				**540 800**
Julius Glaser	Project grant	2001-1612	Studies of speciation, structure and dynamics of coordination compounds	650 000	650 000				
		2004-4474	Studies of speciation, structure and dynamics of coordination compounds			675 000	675 000	675 000	**3 325 000**
Mikael Håkansson	Project grant	2003-4259	Absolute asymmetric synthesis		405 000	405 000	405 000		
		2006-3939	Absolute Asymmetric Synthesis					600 000	**1 815 000**
Ulf Jansson	Project grant	2002-4353	Synthesis and characterization of new MAX-phases	608 400	608 400	608 400			
		2005-6182	Synthesis and characterization of complex carbide films				607 500	607 500	**3 040 200**
Lars-Gunnar Johansson	Project grant	2001-2074	The atmospheric corrosion of Al and Mg alloys	520 000	520 000				
		2003-4181	Synthesis of high temperature superconductors and other perovskite oxides with a strong coupling between charge, lattice and spin degrees of freedom: The reation between structure and properties		405 000	405 000	405 000		**2 255 000**

Name	Type of funding	Reg. No.	Project title	2003	2004	2005	2006	2007	Total
Mats Johnsson	Project grant	2001-1778	Synthesis and characterisation of materials having low-dimensional magnetic couplings	260 000					
		2003-2924	Synthesis and characterisation of low-dimensional materials		594 000	594 000			
		2005-5428	Synthesis and characterisation of low-dimensional materials				610 000	610 000	**2 668 000**
Vadim Kessler	Project grant	2001-3352	Metallosiloxanes - molecular structure models of nanoporous materials: synthesis, structure and reactivity studies	520 000	520 000				
		2005-3435	Molecular precursor and molecular models of nanoporous materials				610 000	610 000	**2 260 000**
Lars Kloo	Project grant	2002-3715	Development of Electrolytes for Photoelectrochemical Solar Cells	811 200	540 800				
		2002-3733	The Synthesis and Characterisation of Cluster and Low-dimensional Compounds	270 400	811 200	811 200			
		2004-4509	Ionic Liquid Electrolytes for Photoelectrochemical Solar Cells			607 500			
		2005-5447	New Media for Clusters, Low-dimensional Materials and Electrolytes				1 100 000	1 100 000	
	PhD student	2002-889	Synthesis, structure and bonding in clusters Syntes, struktur och bindning i kluster	395 200					**6 447 500**
Sven Lidin	Project grant	2002-4692	The many phases of intermetallics	1 014 000	1 115 400	1 115 400			
		2005-3439	The many phases of intermetallics				1 100 000	1 100 000	**5 444 800**

Name	Type of funding	Reg. No.	Project title	2003	2004	2005	2006	2007	Total
Jan-Olle Malm	Project grant	2006-3619	Nanocrystallography based on electron microscopy methods					743 900	**743 900**
Ebbe Nordlander	Project grant	2002-3904	Biomimetic/bioinorganic and organometallic chemistry of transition elements - synthesis and reactivity studies of mono- and polynuclear transition metal complexes	608 400	608 400	608 400			
		2005-5486	Biomimetic/bioinorganic and organometallic chemistry of transition elements - synthesis and reactivity studies of mono- and polynuclear transition metal complexes				675 000	675 000	**3 175 200**
Ingmar Persson	Project grant	2001-1774	Structure, Bonding and Thermodynamics of Metal Ions and Complexes in Solvents with Special Coordination Properties	416 000	416 000				
		2004-4600	Structure, Bonding and Thermodynamics of Metal Ions, Anions and Complexes in Solvents with Special Properties at Coordination			472 500	472 500	472 500	**2 249 500**
Per Persson	Project grant	2003-3439	Molecular studies of processes controlling the speciation, mobility and availability of phosphates and phosphonates in soils and surface waters		607 500	607 500	607 500		
		2003-3700	Coordination chemistry at the interface between aqueous solutions and micro- and nano-sized metal oxide particles		337 500	337 500	337 500		
		2006-5152	The importance of interfacial reactions in the biogeochemical cycle of phosphorus					742 500	**3 577 500**

Name	Type of funding	Reg. No.	Project title	2003	2004	2005	2006	2007	Total
Magnus Sandström	Project grant	2003-3062	Coordination and chemical bonding in solvated complexes and ions, especially by means of x-ray absorption spectroscopy		540 000	540 000	540 000		
		2006-4061	Coordination and chemical bonding in solvated complexes and ions, especially by means of x-ray absorption spectroscopy					550 000	**2 170 000**
Staffan Sjöberg	Project grant	K 5104-20005180/2000	Chemical Speciation in Solution and the Solid/Solution Interface. Models and Modelling	433 900					
		2003-3049	Chemical speciation in solution and at solid/solution interfaces. Models and modelling		607 500	607 500	607 500		
		2006-4068	Chemical speciation in solution and at solid - solution interfaces. Models and modelling					550 000	**2 806 400**
Gunnar Svensson	Project grant	2001-2033	Carbon for energy storage	351 000					
		2003-3114	Nano-porous carbon for energy storage		607 500	607 500	607 500		**2 173 500**
Jan-Erik Svensson	Project grant	2002-5443	Active Corrosion of Fe-Cr alloys at High Temperature - Chemical Breakdown of Chromia-containing Scales by the Formation of Gaseous Species	540 800	540 800	540 800			**1 622 400**
Zoltán Szabó	Project grant	2002-3742	Photochemical reactions of the uranyl ion	270 400	270 400				**540 800**

Name	Type of funding	Reg. No.	Project title	2003	2004	2005	2006	2007	Total
Reine Wallenberg	Project grant	2001-1986	Fabrication, characterization and applications of nanowhiskers	585 000	585 000				
		2003-3007	Nanostructured functional materials		675 000				
		2004-4757	Nanostructured Functional Materials			1 520 000	1 350 000	1 350 000	
	Senior Research position	2002-1988	Inorganic synthesis and characterisation of clusters	884 960					**6 949 960**
Ola Wendt	Project grant	2001-1442	Organotransition metal chemistry. Reaction mechanisms in homogeneous catalysis	299 000					
		2002-1503	Metal-Organic Chemistry, particularly reaction mechanisms in homogeneous catalysis	343 200					
		2003-3073	Organotransition metal chemistry. Reaction mechanisms in homogeneous catalysis		405 000				
		2004-4761	Organotransition metal chemistry. Reaction mechanisms in homogeneous catalysis			607 500	607 500	607 500	
	Junior Research position	2001-5749	Metal-Organic Chemistry, particularly reaction mecha-nisms in homogeneous catalysis	625 976					
	Senior Research position	2006-486	Activation of small molecules in homogenous catalysis					241 250	**3 736 926**

Name	Type of funding	Reg. No.	Project title	2003	2004	2005	2006	2007	Total
Gunnar Westin	Project grant	2001-2397	New materials designed in hierarchic structures on atom, nano and micro scale	325 000					
		2003-4360	New materials designed in hierarchic structures on atom-, nano- and micro-scale		594 000	594 000	594 000		
		2006-3967	Advanced solution processing of complex materials; from molecules to materials					610 000	
									2 717 000
Xiaodong Zou	Project grant	2001-3355	Smart materials - design of highly specific molecular sieves	520 000	520 000				
		2004-4778	Design of functional porous materials			678 227	607 500	607 500	
	Equipment	2001-3355	Smart materials – design of highly specific molecular sieves (Multiscan CCD camera)	550 000					
									3 483 227
Lars Öhrström	Project grant	2001-3601	3D-Nets with Magnetic Properties or Chiral Porosity – From Fundamental Interactions and Models to Applications	520 000					
		2003-3636	3D-Nets with Magnetic Properties or Chiral Porosity – From Fundamental Interactions and Models to Applications		594 000	594 000	594 000		
	Travel grant	2007-1273	Research collaboration with CEA-Grenoble, use of laboratories					27 000	
									2 329 000
TOTAL				**16 579 276**	**19 079 340**	**18 316 667**	**17 117 600**	**17 051 350**	**88 144 233**

* The table presents the following grants awarded:
Project grants; Travel grants; Research Equipment grants (< 2 million SEK); Grants for Junior Research position; Grants for Senior Research position; Grants for PhD student. The amounts are listed in SEK and are including overhead costs. Research Equipment grants (> 2 million SEK) are not included here.

SAMMANFATTNING PÅ SVENSKA

International Evaluation of Inorganic Chemistry, 2008

Under 2008 har en utvärdering av ämnesområdet oorganisk kemi i Sverige genomförts av en internationell expertpanel. Panelen har bedömt tjugonio forskare och deras forskningsverksamhet som har finansierats av Vetenskapsrådet under åren 2003–2007.

Expertpanelen uttalar sig också om den oorganiska kemin i Sverige sett ur ett internationellt perspektiv, dess styrkor och svagheter, samt hur de senare skulle kunna förbättras. Vidare ger panelen råd om balansen för Vetenskapsrådets projektstöd mellan de olika subdisciplinerna inom oorganisk kemi i Sverige. Slutligen har panelen lämnat ytterligare rekommendationer avseende stöd för grundforskning till forskare i Sverige och råd om balansen mellan olika discipliner inom kemi.

Panelen menar att ett starkt stöd till forskning inom oorganisk kemi är avgörande för framsteg inom andra forskningsområden såsom nanoteknologi, bioteknologi, miljökemi, materialvetenskap och energiforskning. Oorganisk kemi omfattar många ämnesområden och inom forskningen söker man få grundläggande förståelse för struktur hos och bindning i molekyler och material.

I Sverige bedömer panelen att forskningen inom oorganisk kemi som Vetenskapsrådet stöder är solid och av utmärkt kvalitet inom flera subdiscipliner, men att forskningen inte alltid ligger i forskningsfronten. Panelen menar att bidragsmottagarna och produktiviteten i grupperna är bra, mycket bra eller utmärkt, men att relativt få artiklar som baseras på forskningen publiceras i ledande tidskrifter, samt att dessa artiklar i allmänhet inte citeras så mycket. På basis av detta drar expertpanelen slutsatsen att en del bidragsmottagare misslyckas med att tackla problem i forskningsfronten av deras respektive ämnesområden. Panelen noterar också att, förutom inom materialvetenskap och nanovetenskap där Sverige är starkt, behöver den oorganiska kemin stärkas framför allt inom områden såsom koordinationskemi och bio-oorganisk kemi samt områden som är fundamentala för energi- och materialforskning. Man påpekar dock att denna utvärdering inte täcker all forskning inom oorganisk kemi i Sverige, t.ex. forskning som finansieras av andra forskningsfinansiärer, såsom exempelvis av SSF och VINNOVA.

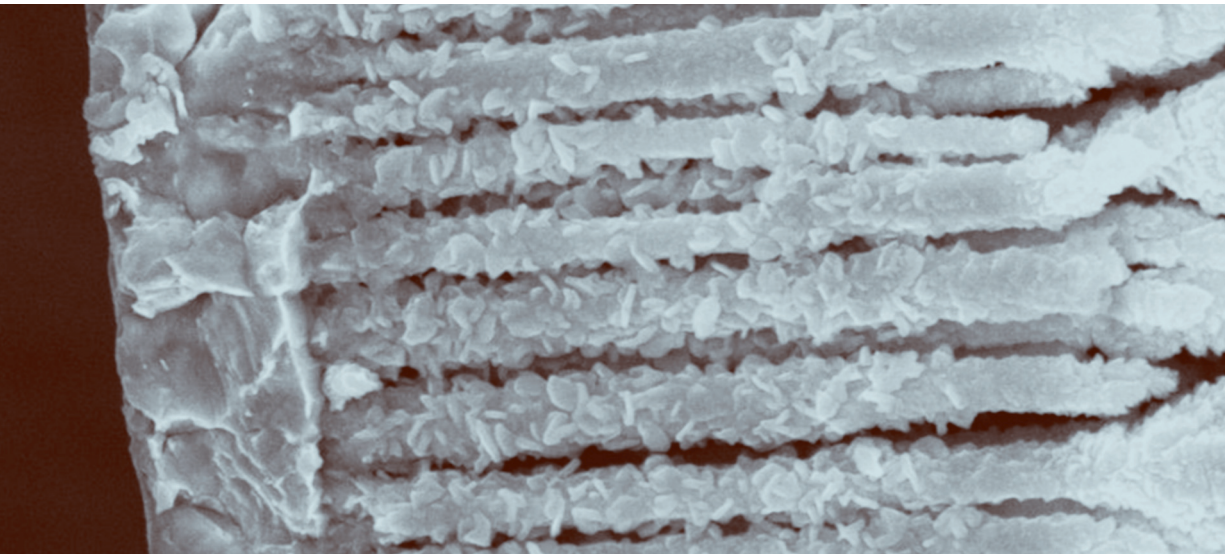
Expertpanelen noterar även att den omorganisation som har skett på flera universitet/högskolor har lett till att institutioner för oorganisk kemi har försvunnit och att professurer inom oorganisk kemi mycket sällan utannonseras eller återbesätts då ämnesföreträdare går i pension. Detta har skapat betydande frustration hos forskarna och en osäkerhet om hur det ska bli för den oorganiska kemin i Sverige. Panelen menar att denna försvagning av oorganisk kemi i Sverige är i stark kontrast till vad som görs internationellt. Man menar att kemi, och då särskilt oorganisk kemi, är grundläggande för att hjälpa till med att lösa dagens energiproblem. Genom att försumma forskningen inom oorganisk kemi kommer Sverige att utestängas från att delta i dessa strävanden. Panelen rekommenderar att det noga tänks igenom huruvida man ska upprusta och till och med öka antalet fullt finansierade laboratorier inom oorganisk kemi i Sverige för att behålla balansen mellan existerande forskningsinsatser och tillåta att utveckling sker inom nya viktiga forskningsinriktningar. Vidare rekommenderar panelen att ökad specialisering inom olika delar av oorganisk kemi främjas hos universiteten/högskolorna i Sverige.

Flertalet av de utvärderade bidragsmottagarna är oroade över hur de ska finansiera sin egen lön för att kunna genomföra sin forskning. Vanligen används delar av Vetenskapsrådets forskningsbidrag till att finansiera forskarnas egna löner. Panelen förvånas av hur liten del av lönen för forskning universiteten/högskolorna finansierar. Man menar att denna situation är skadlig och att omedelbara förändringar behövs samt att en hållbar lösning i ett längre perspektiv också ska sökas.

Panelen ser också behov av en betydande ökning av storleken på Vetenskapsrådets beviljade forskningsbidrag och en modell som gör det möjligt för olika forskningsgrupper att bilda team som tillsammans dels kan söka större bidrag för grundforskning, dels finna och utveckla gemensamma strategier för undervisning och forskning inom oorganisk kemi i Sverige.

Twenty-nine scientists and their research supported by the Swedish Research Council (at eight universities) in the field of Inorganic Chemistry are reviewed by an international expert panel. Each review in this report includes an evaluation of the research and recommendations based on the work accomplished over the past five years (2003–07) and the proposed future research.

The expert panel also expresses its international viewpoints on the status of Inorganic Chemistry research in Sweden, the strengths of the research topic and how to enhance its level and internal coherence. In addition, the panel advises on the balance of research supported by the Swedish Research Council within the various subdisciplines of Inorganic Chemistry. Finally, the panel makes some additional recommendations on research funding to scientists in Sweden, and gives advice on the balance among the various fields of Chemistry.



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The Swedish Research Council is a government agency that provides funding for basic research of the highest scientific quality in all disciplinary domains. Besides research funding, the agency works with strategy, analysis, and research communication. The objective is for Sweden to be a leading research nation.

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