# *Evaluation of Estonian Research*

## *- Atomic, Molecular, and Optical Physics -*

Report to the Estonian Science Fund Council

by

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February 1992

The authors of this report were appointed for the purpose of this evaluation by the Swedish Natural Science Research Council.

NFR Naturvetenskapliga forskningsrådet
Swedish Natural Science Research Council

## Foreword

Several Swedish organizations have been asked to take part in a general evaluation of all research performed at academic institutions in Estonia. NFR has agreed to organize the evaluation of Estonian research within the field of natural science. This report has been prepared according to an agreement between the Estonian Science Fund Council and the Swedish Natural Science Research Council (NFR).

During the spring of 1991 Estonian scientists completed reports on their research which were sent to NFR. These reports have subsequently been distributed among 14 Swedish evaluation groups. In total about 40 Swedish scientists are engaged in the evaluations. The groups are making site visits to the Estonian laboratories and institutes during 1991/92 to discuss the research performed, the plans for future activities and to get information about the working conditions, experimental facilities, financial resources etc. Each group has been instructed to produce a report assessing its particular research area.

This report concerns the sub-field of atomic, molecular and optical physics and will eventually be a part of an extensive report covering all Estonian research in natural science.

The organization of the site visits is done in close cooperation with the Estonian Science Fund Council. Although difficult times prevail in Estonia the site visits performed so far have been successful. The NFR is grateful to the Estonian Science Fund Council for its efforts to handle all practical matters in connection with these visits.

The NFR is also grateful to the Swedish scientists who with enthusiasm and great skill have taken part in the demanding evaluation work.

Finally, the Council wishes to express its sincere hope that this evaluation report will contribute to a further positive development and strengthening of Estonian science.

Carl Nordling
Secretary General

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## INTRODUCTION

The Estonian Science Fund Council has instructed Estonian scientists in the field of Atomic, Molecular and Optical Physics to prepare reports concerning their research activities during the last 5 years. These reports were completed during the spring of 1991 and dealt with the following points:

- project leader(s)
- short description of the objectives
- summary of results
- summary of resources
- scientific staff and their qualifications
- list of publications
- dissertations
- scientific meetings organized
- prognosis of the future development of the project

In most cases the reports were accompanied by reprints of scientific publications written in English and Russian.

In July 1991 the reports were sent to NFR and during the autumn the evaluators received the reports. A site visit by the evaluators to the relevant Estonian research institutions was done in the period December 15-18 1991. The Estonian Science Fund Council had appointed Drs Mati Karelson and Jüri Tamm as organizers and contact persons for this evaluation. Dr Jüri Tamm was the contact person during the entire site-visit of the Evaluation Group.

This report was drafted in January 1992 and was finally approved by the Evaluation Group in a meeting in Stockholm on February 20. Dr Jüri Tamm and Dr Lars Gidefeldt from NFR took part in this meeting. However, the Evaluation Group itself takes full responsibility for the entire report.

## ACKNOWLEDGEMENTS

This evaluation would not have been possible without the good cooperation of the interviewed scientists and the most generous help of Dr Jüri Tamm. We were met with great hospitality. We hope that our small contribution may help our scientific colleagues in Estonia.

## GENERAL COMMENTS ON ATOMIC, MOLECULAR AND OPTICAL PHYSICS

The goals of atomic, molecular and optical physics (AMO) are to understand the structure of matter and how matter evolves at the atomic and molecular level, to understand light in its different manifestations and how it interacts with matter, and to create new techniques and devices. AMO physics provides physical data that are of vital interest to other areas of science and technology and it plays an active role in educating scientists at the undergraduate and graduate levels.

The research activities in AMO physics in Estonia cover only a small part of the total field. This is natural for a small country like Estonia. Theoretical research seems to have a smaller activity than expected compared to the efforts in experimental research seen in an international perspective. Furthermore, it appears as if the division of physics in Estonia, and maybe in the former Soviet Union as a whole, is somewhat different from how physics is split into sub-fields in Western countries. This is, however, not a concern, but should be kept in mind when the evaluation is read.

Atomic physics appears to be almost non-existent in Estonia. The only activities which marginally falls within the domain of atomic physics are the investigations of discharge laser plasmas at the Institute of Physics in Tartu. There is no kernel of scientists around which atomic physics could be expanded.

Molecular physics is carried out at a number of places in Estonia, both in Tallinn and in Tartu, and includes both modern developments such as laser spectroscopy in jet cold expansions as well as more traditional photoelectron spectroscopy. Some of the molecular physics work is clearly directed towards applications. This is not unusual seen in an international perspective.

Optics is well represented. The main emphasis is on the understanding and development of gas lasers, development of VUV instrumentation and radiation sources, and production of optical elements. There is a strong link between basic research in optics and commercial enterprises. This link will probably be instrumental for help supporting the basic research during the time when Estonian research is transformed.

The quality of atomic, molecular and optical physics in Estonia ranges from very good to mediocre. In this respect, Estonia is not different from any other country with the exception that Estonia lacks the top notch groups one can find in the Western countries. In order to increase their international visibility, the research groups must publish in English in major international journals. For some groups this does not represent a problem, for others it is a formidable challenge. International collaboration should be increased.

It is reasonable that a small country like Estonia concentrate its resources in a small number of areas. The most sensible policy is to identify the strongest scientists and concentrate the resources on them. Of course, this policy should not be carried too far, since it is also desirable, for a number of reasons, to maintain a presence in several areas. It is also important that research groups receiving support are reasonable large and not allowed to drop below a sub-critical size. In order to vitalize the field with younger scientists a better collaboration between University and the Academy should be pursued. Presently, the most active research in AMO physics is carried out at the Academy and the scientists have no connection with teaching at the universities. The fruitful development of small technical companies as spin off to a scientific project is positive and could even further stimulate creative students to enter the research field if the links between University and the Academy were properly established.

EVALUATION OF RESEARCH GROUPS

**Juhan Subbi, Cand Sc**
**Laboratory of Chemical Physics**
**Institute of Chemical Physics and Biophysics**
**Estonian Academy of Sciences**
**Tallinn**

*Investigation of Vibronic Interaction and Vibrational Relaxation in Molecules Isolated in Supersonic Jet and Low Temperature Matrices*

## Principal Activities

J Subbi has mainly concerned himself with laser spectroscopy of 1,4DAQ (quinizarin, $C_{14}H_8O_4$) and other fairly large organic molecules in supersonic jet cooled expansions. These molecules act as model systems for investigation of various effects connected to the interplay between molecular structure and reactivity. Subbi has worked both in the frequency- and time-domain and investigated effects of vibronic coupling, normal mode mixing and vibrational relaxation. In addition to this he has also developed a theory for calculating multidimensional Franck-Condon factors for electronic transitions in the case of strong normal coordinate coupling. Subbi has on several occasions published his work, also as sole author, in major international journals within his sub-field.

The Evaluation Group did unfortunately not meet J Subbi during the site visit in Tallinn. It was further informed that J Subbi now has a new project related to the development of a new generation of detectors for LHC. The Evaluation Group is not well-placed to judge the relevance of this project; however, in order to meet endorsement from CERN it will have to stand up against a fierce international competition. The laboratory is well equipped with commercial laser systems, multichannel detectors and data acquisition systems.

## Evaluation

J Subbi has clearly demonstrated that he is capable to do very good molecular physics work. He has successfully worked with both experiments and theory. He has demonstrated flexibility to meet the future.

## Recommendations

Support for J Subbi's future molecular physics work is most strongly recommended. He is himself in the best position to judge if this should be the type of basic work he has carried out so far or in the form of the more applied work related to the CERN project. J Subbi should have at least one or two graduate students.

**Valdur Tiit**
**Laboratory of Equipment Development**
**Institute of Physics**
**Estonian Academy of Sciences**
**Tartu**

*Instrumentation for VUV and UV Spectroscopy and Its Applications*

## Principal Activities

The work of this group has spanned over more than three decades with development and manufacturing of instruments. During this long time the group has delivered several spectroscopic instruments which have been successfully used in various applications, e.g., solid state physics and space sciences. Some of the instruments, in particular the double vacuum monochromator, have been successfully developed (and patented in several countries) and observed internationally. On the detector side calibration techniques for more traditional detectors have been developed. On the radiation source side, a compact laboratory synchrotron radiation source has been under development for the last five years with the goal to develop a radiation source in the UV which can be housed in a traditional research laboratory in contrast to otherwise successfully developed synchrotron radiation storage rings (which are also in use in Russia).

Presently, the instrumental work is limited to manufacturing a few instruments, e.g., a double vacuum monochromator for a laboratory in Kiev, and a reflectometer. Most of the new design and manufacturing of modern instruments is now carried out in the technical companies which have evolved out of the work of this group. The group leader, V Tiit, is now close to retirement and there is no strong group of active research scientists to carry on the work. Rather it seems that the active scientists, who started in this group and are known internationally, now work in the technical companies.

## Evaluation

The work in this group is fair, as the group does not seem to have been able to follow the very rapid development in this field during the last decade. The work of the group has been based on collaboration with (former) Soviet groups and there are no firm links with other international groups. The project on developing a laboratory radiation source should, if continued, be carried out in collaboration with some of the many very active international groups.

## Recommendations

Support for this group is not recommended. There is no group of young scientists to reactivate the research in the group and the few remaining scientists could possibly be engaged in similar activities within the technical companies which exist in close liaison with the group.

**Aleksei Treshchalov, Cand Sc**
**Laboratory of Laser Technique**
**Institute of Physics**
**Estonian Academy of Sciences**
**Tartu**

*Spectroscopic Diagnostics of Plasmo-Chemical Processes in the Active Media of Discharge-Pumped Gas Lasers*

## Principal Activities

This project concerns the study of atomic and molecular processes in the active media of discharge-pumped gas lasers. The research is pursued both with experimental work using dye laser probe techniques combined with advanced spectroscopy and with theoretical modelling of the reaction kinetics in the active media. In the probe experiments temporally and spatially resolved studies have revealed the importance of ion-atom processes in the creation of excited states of the active excimer. These results are of importance for understanding the reaction mechanism in the excimer laser. The results have been published in international journals and have been presented at several international conferences. Measurements of rate coefficients in the active media coupled with theoretical modelling of gas dynamics have furthermore resulted in an increased understanding of the plasmo-chemical processes of gas lasers with the possibility to optimise the design of the active media and the discharge to achieve high gain lasers. The research is also the basis for development of new, compact gas lasers which the group has successfully pursued. Very sensitive diagnostic techniques have been developed to be able to measure minute concentrations, down to $10^{-11}$, in the active media and several combinations of gases are studied to optimise the discharge.

## Evaluation

This project is scientifically very good and constitutes the main research for the group led by A Treshchalov and his coworkers, V Peet, E Slivinskij and R Sorkina (the latter presently in the Netherlands in a scientific collabortive program). The group has developed its own profile and its results are presented at international conferences and in international journals. The group has also hosted several scientific meetings and A Treshchalov has been awarded with several prices for his research. The project has also attracted several Diploma and PhD students. The leader, A Treshchalov, is a dynamic and a very competent physicist with great experience in the field and he has also shown to be very capable of developing a sound scientific program with good collaborators.

## Recommendations

Support for this group is most strongly recommended since scientific quality of the research is very good. The structure of the group, with senior and junior research staff and students, is very healthy and the group could very well be larger. It is also very important that the group gets sufficient technical staff support. In a highly active experimental program like this one, strong support is needed for equipment and running costs in order to be able to pursue the very good research program.

**Aleksei Treshchalov, Cand Sc**
**Laboratory of Laser Technique**
**Institute of Physics**
**Estonian Academy Sciences**
**Tartu**

*High Resolution Laser Spectroscopy of Jet-Cooled Molecules*

## Principal Activities

About four years ago A Treshchalov and his young co-workers, S Tsarenko and E Jalviste, started a research program aiming at laser spectroscopy of jet-cooled molecules. The supersonic beam equipment they have built is fairly standard; the excimer pumped dye lasers are combined with frequency doubling in order to cover the UV spectral range. In the initial phase the group investigated quinizarin and some other organic molecules. More recently they have recorded fluorescence spectra of benzotriazole ($C_6H_5N_3$). They have tentatively suggested that different tautomers (dynamic isomers) correspond to the upper and lower electronic states involved in the observed transition. Publication so far has been restricted to conference proceedings and journals of the USSR and Estonia.

Future directions involve development of two-photon ionization spectroscopy and the "pump-dump" technique, spectroscopy of biologically important molecules and, in this connection, analytical detection of small amounts of substances in drugs, food products etc.

## Evaluation

The work by A Treshchalov and co-workers is good. It makes sense for a group leader with several projects aiming at development of lasers to have at least one project directed towards the application of lasers and laser spectroscopy.

## Recommendations

A Treshchalov is a very competent scientist with well thought ideas how he should meet the future. The plans to use the supersonic beam apparatus for analytical purposes sound interesting and are well worth to pursue. With increased spectral resolution it is definitely possible for the group to make an impact in the field of spectroscopy of large molecules. Support for this project is strongly recommended. Future results of this group should be published in major international journals.

**Aleksei Treshchalov, Cand Sc**
**Institute of Physics**
**Estonian Academy of Sciences**
**Tartu**

*Development of High-Efficiency Excimer Laser Systems*

## Principal Activities

The main emphasis of this project is to develop new laser systems which can be introduced on an international market. However, the project also includes new scientific work to develop laser systems into the VUV regime using resonant mixing and frequency tripling of dye lasers. Thus, based on the scientific studies of plasmo-chemical processes, an advanced engineering effort has to take place to design and to construct laser systems which are high-efficient, compact and reliable. In these laser systems all the components are developed and tested at the Institute of Physics, including the design and manufacturing of optical elements (A Kasikov). The final product is assembled in collaboration with local technical companies. Several of these laser systems have been spread to other research groups and some have also been sold. Presently, an effort is made to introduce a compact excimer laser system on the international market with the goal to sell seven to ten systems during the next year. Thus, the work is carried out in a constructive way with technical companies and the success of the work is crucially dependent on the possibility to manufacture and sell on the competitive international market as well as to find optimum design criteria for new applications of the laser systems in e.g., medicine, chemical and technical industry, and environmental studies.

## Evaluation

The Evaluation Group did not visit any of the companies involved and the evaluation is based on the visit with Treshchalov's group where several of the laser systems are in use and under further development. This research is good to very good and seems to be able to stimulate fruitfully the research team into international collaborations. The possibility to work in a synergetic manner with local technical companies also gives the group possibility to extra technical support which now seems to be on a too low level. The work on development of laser systems into the VUV is good but not unique and could benefit from international collaboration with groups in the same field which exist in several places in Europe.

## Recommendations

Support for this project is strongly recommended and should be linked to the possible economic profit gained from the final product. A project like this, a "university-industry" collaboration, is highly attractive for a small country like Estonia and could give the basic research a firmer support. Furthermore, such a project is automatically evaluated by the possible success of the final products but the program needs to be firmly supported in the development phase.

**Jaan Villem**
**Niina Villem**
**Department of Experimental Physics**
**Tartu University**

*Study of Materials Using the Method of Photoelectron Spectroscopy*

## Principal Activities

J Villem learned photoelectron spectroscopy (PE) from F Vilesov, one of the founders of PE of the outer shell. Together with N Villem he has studied organic molecules in gas phase by means of photoelectron spectroscopy. Because of the great variety of molecular orbitals and large number of vibrational degrees of freedom in organic molecules, the Villems have studied groups of homologous compounds in order to extract information that would elude a detailed investigation of an isolated system. For example, photoelectron spectra of eight fluoro-derivatives of benzoyl chloride have been recorded. From these spectra the influence of F-substitutions have been elucidated.

The work of this group falls entirely within the domain of traditional UV photoelectron spectroscopy. Very little work has been put into improving the photoelectron spectrometer and the resolution is now an order of magnitude lower than state-of-the-art. Publications are invariably in Russian.

## Evaluation

Since the works of the Villems are published in Russian it should be emphasized that the Evaluation Group has not taken part of their original publications. With this reservation we rank their work as fair. They have a very low international visibility.

## Recommendations

We recommend no further support for this group (apart from salaries). The Villems could be integrated in the undergraduate teaching. The photoelectron spectrometer should be useful for undergraduate laborations or for Diploma works.

## APPENDIX

### Background of evaluators

**Elisabeth Källne**

Docent in Physics, presently at the Department of Physics I, Royal Institute of Technology, Stockholm. Her research interests concern structure and dynamics of atoms, ions and molecules; low energy collisions of photons, electrons, atoms and ions; atomic and molecular processes in hot plasmas with applications to fusion and astrophysical research. She holds a special research position in Low Energy Collision Physics at the Swedish Natural Science Research Council.

**Mats Larsson**

Docent in Physics, presently at the Department of Physics I, Royal Institute of Technology, Stockholm. His current research interests are in spectroscopy of transient molecules and ions, and low energy electron-ion collisions. He holds a special research position in Atomic and Molecular Physics at the Swedish Natural Science Research Council.