Farewell Lecture

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May 4, 2026

Title page

Already as a child I was a little boy. I was curious and wanted to know, which is a good start for a researcher. I said ”eidee” meaning ”what is that” before I could speak properly.

Childhood

I was born on December 22, 1957. My father was a fisherman until 1959. My father’s best friend had emigrated to California a few years earlier. He had founded a company and needed reliable coworkers. He asked my father to join him. My father hesitated because he had two small boys. He decided to stay in Finland. He started with my mother a mink farm in 1959. It was a family business involving everybody in the family. Without that choice, I would not be where I am today. I became a strong small boy as mink farmer. I remember that I fed the minks on Sundays carrying boxes with 40 kg mink food when I was less than 10 years old. The small and youngest boy was arm wrestling master. The pictures to the left show me when I was 7 months and 6.5 years old. The pictures to the right show my parents returning with lots of baltic herring as well as me and my older brother Jan (b. 1954). The picture of the childhood home is taken in 1997.

School

I was born in Vexala, a small village with about 300 inhabitants. Munsala was the municipality, which in 1975 became part of Nykarleby. This is one of the most Swedish-speaking areas in Finland. Vexala at the west coast is marked on the map to the right. Helsinki is marked at the south coast of Finland. I began in Vexala public school in the fall 1964. I visited the school before that because I was home alone and liked learning something new. I was called Kivikoski in the village after a quiz master on TV. The school picture is taken in May 1965. The yellow school building is behind us on the photo. The school had seven classes with six pupils in each class. We had two teachers and a cook. The school was closed in 1986. The pupils were moved to Munsala, which was the center of the municipality. I moved to the private intermediate school Nykarleby Samskola and continued to the high school Nykarleby Gymnasium, which was in practice the same school. Now it is called Topelius Gymnasium after Zacharias Topelius, who was born in Nykarleby. I got my high-school diploma in 1976.

University Studies, part 1

University studies were rare among young people in Vexala. Thus, there was a shortage of role models. One of my older cousins and a girl next door began to study at Åbo Akademi University a few years before me. My older brother Jan studied IT at Umeå University. He returned home and continued the fur farm when our father retired. Ten years later he quit being a fur farmer and started to work in IT until retirement. Karl-Gustav Fogel was Professor of Physics and Rector of the Åbo Akademi Unversity. He was born in Vexala and had his summer place near my childhood home. He was my father’s second cousin. Kurt Nyholm was Professor of Germanic Philology and Rector of the Åbo Akademi Unversity. He was born in Munsala and had his summer place in Vexala 1 km away from my childhood home. Honestly, I knew very little about jobs after an academic degree. Since I liked chemistry, mathematics and physics, I thought that education in engineering could bring a nice job. A future employer could be the nearby paper mill in Jakobstad. I was also fascinated by catalysis. I began to study Chemical Engineering at Åbo Akademi University in 1976. Pulp and paper chemistry was the primary aim. However, I disliked some process

engineering courses and switched to chemical engineering to avoid them. After two years of studies (Lilla Dippen), I decided to take more courses than the obligatory ones. After four years, I had taken almost all courses that were available. I was curious and wanted to know. I did not take the advanced courses in process engineering and biochemistry.

University Studies, part 2

I decided to take couses in quantum chemistry lectured by Professor Pekka Pyykkö. In parallel, I did my M.Sc. thesis work in heterogenous catalysis with Professor Lars-Eric Lindfors. The title of my M.Sc. thesis work (1981) was ”Oxidation av Kolmonoxid över Nickeloxid Katalysatorer”. I was interested in PhD studies and asked Professor Lindfors whether he had funding for a PhD student. The answer was no. I then asked Professor Pekka Pyykkö. His answer was yes. I ended up doing a degree in Physical Chemistry with Chemical Engineering as the minor subject. I became Licentiate of Technology in 1983 at Åbo Akademi University. We built a spinning-basket reactor, synthesized a zeolite catalyst and run methanol to gasolin (MTG) reactions. I showed a poster ”Conversion of Methanol to Hydrocarbons over a ZSM-5 Zeolite Catalyst in a Spinning Basket Reactor” at the Nordic Conference on Surface Science in Tampere, 1982. A paper was submitted but I do not know what happened to it. It was never published. Professor Pyykkö offered two topics: ”Numerical Electronic Structure Methods” and ”Computational Studies of NMR Chemical Shifts”. I chose NMR without understanding that the question was retorical. He gave a copy of the article below by R. M. Stevens, R. M. Pitzer and W. N. Lipscomb. This article is relevant in my recent research, where we study spatial contributions to NMR chemical shifts. My PhD thesis work was about numerical electronic structure methods.

Entering the Quantum Chemistry Community at Åbo Akademi

The picture to the left is taken at a group meeting at the Åbo Akademi University when Jean-Paul Desclaux was visiting. Arlen Viste was guest researcher from USA on sabbatical leave. From left to right stand Dage Sundholm, Matti Hotokka, Arlen Viste, Pekka Pyykkö, Jean-Paul Desclaux and Leif Laaksonen. The lower picture to the left was taken when I participated in the International Congress of Quantum Chemistry (1982) in Uppsala. Matti Hotokka, Dage Sundholm and Leif Laaksonen sit on the park bench. The International Congress of Quantum Chemistry (ICQC) in Uppsala in 1982 was my first quantum chemistry conference. After ICQC, we organized the satellite conference Relativistic Effects in Quantum Chemistry in Åbo. The conference picture is shown to the right. I am the third one from left in the middle row sitting between Werner Kutzelnigg and Ian Grant.

Moving to Helsinki

The numercial project was in close collaboration with Leif Laaksonen, who defended his thesis ”Two-dimensional fully numerical solutions of molecular Schrödinger equations”” at Åbo Akademi University in 1983. The title of my Licentiate of Technology thesis was ”Tvådimensionella Numeriska Lösningar till Molekylära Hartree-Fock och Hartree-Fock-Slater Ekvationer” (1983). In January 1985, I officially moved and became a PhD student at the University of Helsinki, where I defended my thesis in September 1985. The title of my thesis was ”Applications of Fully Numerical Two-Dimensional Self-Consistent Methods on Diatomic Molecules”. The picture to the left shows me defending my PhD thesis. In the middle picture we see my opponent Jean-Paul Desclaux, custos Pekka Pyykkö, and me. A photo of the cover page of my thesis is shown in the right picture. The PhD was not the end, it was the end of the beginning (Winston Churchill).

My Family

Behind every successful man there is a surprised woman. Maj-Len and I married in February 1986 when I did my military service. We have two boys, who were traveling with us until they were grown-ups. Mathias was born in 1987 in Lund, when I was post-doc there and Johnny was born in 1989 in Helsinki, when we were back home from Lund. Mathias is an IT expert working with machine learning for a start-up company in München. He is

married to Merve and they have a daughter Aylin, now 21 months old. Johnny is medical doctor and has a PhD. He is rheumatologist and works at the University of Helsinki. He lives together with Charlotta. The photo to the left shows the newly married couple (1986). The next photo from left shows the family when Johnny defended his thesis in 2019. The next photo shows Johnny and Charlotta (2024). The rightmost photo shows Mathias and Merve with their daugther Aylin (2025).

Lund University (1986-88)

Björn Roos was my boss at Lund University. He appreciated that I worked with Jeppe Olsen, who was the bright rising star. He was one of the most talented quantum chemists in the beginning of his career. Jeppe Olsen became professor at Aarhus University. He is now retired. I was lucky to meet him. He was the perfect supervisor even though he was only 1.5 years older than me. In my PhD thesis work, I used finite differences (FD). In Lund, I became wiser and implemented an finite element approach (FE). The matrices are denser when using FE but they are symmetric. I developed an algorithm to solve FE equations and used it in the new 2D-FE program for calculating the electronic structure of diatomic molecules. We combined it with configuration interaction (CI) and did orbital optimization, that is, complete-active-space self-consistent-field (CASSCF) calculations. The only paper was published in Proceedings of NATO Advanced Research Workshop, which was held in Versailles in 1988. We also developed a 1D-FE program (LUCAS), which was a similar program for atomic structure calculations and decided to put the efforts on that. We used the LUCAS program on atoms. The first paper was published in 1990. We published 25 LUCAS papers. It was the best nonrelativistic atomic structure program until Charlotta Froese-Fischer realized that they have to improve their code to be in the lead. I also realized that I will never get a permanent position based on 1D and 2D numerical solutions of Schrödinger equations on atoms and diatomic molecules. I am a chemist and atoms are physics. No way! Nanotechnology was the new scientific field because one could see with atomic resolution. Atomic physics had no future in the 1990:ies, nanotechnology came and it was time to move on.

University of Helsinki (1988-93)

I had a Laboratory instructor position as background job (1986-1995). I was on leave most of the time. For example when I was in Lund and had positions at the Academy of Finland (AKA). My PhD studies were supported by Pekka's AKA project. I had AKA positions in 1990-91 and in 1992-97. My salary was mainly paid from AKA grants in 1981-85, AKA research positions 1990-97, and AKA grants in 1999-2010. I have had continuous AKA projects from 2002 until the fall 2025. I was twice in the final for Academy Professor positions. The Academy of Finland has always been very kind to me, even though "You Can't Always Get What You Want" (Rolling Stones). When I got the 5-year AKA researcher position in 1992, it was time to go abroad again.

Aarhus University (1993)

At scientific meetings in Nordic countries, one heard a lot about "Response Theory". I did not know it well and decided to visit Poul Jørgensen in Aarhus to learn more about it. Maj-Len and I packed our bags and moved in 1993 to Århus with the 4 and 6 years old boys. Poul Jørgensen developed quadratic response methods, which could be used for calculating two-photon absorption spectra. The third member in the project was Antonio Rizzo from CNR in Pisa. Antonio was the master of theoretical spectroscopy. Maria Göppert-Mayer developed the theory of two-photon absorption in her PhD thesis and published it in 1931. It could not be tested before lasers were invented in 1960. The first two-photon absorption experiment was performed in 1961 showing that she was right. This could have been her second Nobel Prize. The two-photon spectrum of Argon was measured in 1981 and we calculated it in 1993. We were lucky, the agreement was perfect. We also studied the two-photon absorption spectrum of carbon monoxide.

University of Karlsruhe, TH (1993), part 1

In the beginning of 1994 we moved to Karlsruhe, where Reinhart Ahlrichs and his group developed the Turbomole program for calculations on large molecules. I was lucky again, I was well adopted by his group. Even though, I did not do what was planned, Ahlrichs supported my independence. It was a fantastic group with young researchers that became good friends and also family friends. Marco Häser had developed the direct SCF program of Turbomole. He was the Turbomole master. He was back after his postdoctoral time with Jan Almlöf in Minnesota. Resolution of the identity was the latest news. Jürgen Gauss was habilitand developing computational methods to calculate NMR chemical shifts. He is now professor in Mainz. Ansgar Schäfer was doctoral student developing basis sets. He has now a high position at BASF. Christian Ochsenfeld was doctoral student performing calculations on sodium chloride clusters. He is now professor at LMU in Munich. There were many other young researchers in the Ahlrichs group. The structure of the group surprised. Der Chef (Ahlrichs), two habilitands and lots of PhD and MSc students.

University of Karlsruhe, TH (1993), part 2

I worked on my own projects and had collaboration with Jürgen Gauss. I published a few papers, one was a single-author JACS paper. I was able to convince Ahlrichs that he should also be coauthor on the ^{1}H NMR magnetic shielding calculations on H_2 at the coupled-cluster singles and doubles (CCSD) level, which is also full CI for two-electron systems. I published one paper with Ansgar Schäfer and Jürgen Gauss when I was back home. I did not publish anything with Marco Häser during my time in Karlsruhe. Instead, we were climbing and hiking in the Alps. The photo shows me climbing towards the Marco e Rosa hut near Bernina. I published a paper with Marco Häser in May 1999 when he had been dead for almost two years. I learned how to play Skat, we played it every day in the lunch break.

The Bernina Tour

The big adventure was the Bernina tour. It did not become as planned. That was typical for Marco Häser, ”langweilig” he called traditional routes. When we arrived to the Marco e Rosa hut, they asked how we reached it. Marco told the man at the hut, who replied: That is not possible because it is too much snow. We rested in the hut and planned to climb up to Bernina before noon the next day. The three others in the group did, I slept and rested in the hut. After an early lunch, we continued to the Diavolezza hut. That means that we have to climb up to the Bella Vista ridge before we can climb down towards the Diavolezza hut. One group member became afraid of hights (not me) and we had to secure many times with ropes. We were delayed and reached the ice glacier after 7 pm. It became dark. Marco and Peter discussed how to continue. They could not agree. Marco decided that he and I go to the left and Peter decided to go to the right. We crossed the ice glacier in the darkness and arrived at 10 pm to the other side of it, where we had to climb in moraine because the hiking path was on the top of the moraine wall. It was possible to climb the steep wall because we could make steps in the moraine wall with the crampons. We were hiking along the moraine wall in the darkness with one headlight and reached the hut at 1 am. Marco had been hiking for 20 hours. I had been hiking for only 14 hours. The photos to the right show the happy hikers at the Diavolezza hut. I have not met Peter since we split before crossing the ice glacier because I was sleeping when they arrived at 3 am and I got up at 5 am to hike down to the valley. I took the train to Karlsruhe. Marco Häser died a year later in a hiking accident.

The Mount Timpanogous Tour

A smaller adventure was our tour to mount Timpanogous with Maj-Len and Christian Ochsenfeld. It is a long one-day hike. One can save time by sliding down on the snow field, as you can see on the picture. That was suggested in the guide book. Now it is not recommended anymore. Maj-Len began to slide and I had to follow. I got a Shakleton feeling. We were not screaming, though. It stopped when the slope was less steep before it became steeper and went down to the lake.

Quantum Dots (1999-2003)

Now I was an educated quantum chemist prepared to stand on my own feet. Jukka Tulkki contacted me and asked whether it would be possible to use our computational methods to calculate photoluminescence spectra of semiconductor quantum dots. I discussed it with Jeppe Olsen and we decided to write a new program for interacting electrons and holes. Mats Braskén and Markus Lindberg were experts in the field. We brought our quantum chemistry methods to solid-state physics and they taught us the theory of solid states. Jeppe modified his LUCIA configuration interaction and coupled-cluster program such that it could treat different kinds of quantum particles. I met Stefano Corni in Pisa at a quantum-dot conference. I had funding for a young researcher and he was prepared to come to Helsinki. Stefano Corni was an excellent young researcher. He knew what to do and did it rapidly. Stefano is now professor at University of Padova. We were a perfect team, experts in different research fields and we had an excellent student. We introduced the recombination density matrix concept, which is useful for photoluminescence calculations because its structure is independent of the employed level of theory. We also implemented a method to calculate phonon-relaxation rates. We realized that such calculations are one way to kill a student. Semiconductor quantum dots have a huge number of excited states and the number of phonon-relaxation rate constants scales quadratically with the number of states. One cannot calculate them all. However, we understood from the expression that the phonon-relaxation rate is not relevant for quantum dots. However, for quantum rings, the phonon relaxation might be slower than the electron-hole recombination. We showed that quantum double rings can emit from excited states.

Just for Fun, part 1

Quantum dots studies were fun and useful. I decided to test a few other crazy ideas. I did not like the quasi-relativistic ZORA approach. I developed my own ERA, MERA, IORA and MIORA models as well as how to do perturbation theory on top of them. It was nice work but noone cared because the X2C method was introduced. I walked from Pasila to Kumpula every day and one day I thought that it should be possible to find unique configuration numbers from orbital indices also for bosonic systems. I designed an algorithm and wrote a simple CI program. Tommy Vänskä became a new PhD student. I asked him to rewrite the boson CI program. We studied boson-boson correlation effect using a direct CI approach, which is the same method as used for electrons. It was a nice piece of work. However, noone cared because correlation effects are not very important for bosons with a steric-interation potential. I also thought about superconductivity. How does it actually work, I asked myself. According to the Bardeen-Cooper-Schrieffer (BCS) theory phonons create an attractive potential. Superconductivity had been measured for a few molecules. Thus, one could see something also at the molecular level. Phonons are vibrations that can lead to an attraction between electrons. I showed a possible mechanism. However, I did not obtain any interaction between the electrons.

Just for Fun, part 2

Pekka Pyykkö began to computationally design new molecules. Mikael Johansson used C_{60} as template to design Au_{32}, the golden fullerene. When I visited Barcelona, I saw an object in the basement of Sagrada Familia. I saw an all-carbon structure. When I came home, we had a family project in the kitchen where we folded paper to reproduce the object on the photo. I used a molecular editor to make the molecular structure. I optimized it, calculated its properties and published a paper. I called it Gaudiene (C_{72}). I realized that other all-carbon structures can be constructed using the same design principle. I met Lukas Wirz in New Zealand. He was the master of constructing molecular structures of nano carbon. We made lots of them and published an article together with Peter Schwerdtfeger. Very recently, we constructed molecules with a novel chemical bond. We call it aromatic bonding of antiaromatic rings. It is a delocalized double bond between each pair of rings.

Winter School in Theoretical Chemistry (1985-), part 1

Pekka Pyykkö started the Winter School in Theoretical Chemistry because the number of teachers in theoretical chemistry was not enough the cover the field. It was organized in December because the laboratory had funding

for teaching that had to be used before the end of the year. The school was aimed for students, young and older researchers. Everybody is welcome because it is free. Lecturers covering different aspects of theoretical chemistry were invited. This is an excellent way of bringing novel know-how to Finland. I hope that the Winter School continues and that the young and older researchers understand its importance. Some for me important themes of the Winter School are marked.

Winter School in Theoretical Chemistry (1985-), part 1

I got more responsibilities and freedom to choose topics. Pekka always opened the Winter School until his retirement in 2009. After that I had the full responsibility for a few years. From 2015 until now, my coworkers have taken lots of responsibility. At least the following colleagues have contributed to the organization of the Winter Schools: Mikael Johansson, Michael Patzschke, Carl-Mikael Suomivuori, Ville Kaila, Stefan Taubert, Susi Lehtola, Theo Kurtén, and Juha Vaara. A large number of students have also helped. I hope that I have not forgotten anyone.

Magnetically Induced Current Density Susceptibility (GIMIC) (2004-)

The GIMIC project started in December 2020 during the NMR Winter School. I realized how one could calculate magnetically induced current density susceptibilities using gauge-including atomic orbitals. Jonas Jusélius was my PhD student and wanted a more advance computational method to implement in a computer program. He is now Chief Technology Officer in the Oceanbox company. I was lucky to have a good and motivated student. He wrote the first GIMIC version. Then, he visited Jürgen Gauss in Mainz, who helped with the interface to the Mainz-Austin version of the electronic structure program ACES2 (now called Cfour). The GIMIC project began 25 years ago, the first paper appeared 22 years ago and now it is used all over the world, because we gave it away. We have published more than 100 GIMIC papers. It is free to download including the source code and free to use. Nothing is ready when you have a code that works. Heike Fliegl, Radovan Bast, Jaakko Paaer, Maria Dimitrova, and Rinat Nasibullin have implemented useful features.

GIMIC Reviews and Book Chapters

Vincent Liégeois made the interface to the Gaussian program. The possibility to use it with the Gaussian program increased the popularity of GIMIC. We have used GIMIC in many applications and written book chapters and reviews.

Selection of Recent GIMIC Applications

Raphael Berger contacted me and asked whether Ampere-Maxwell's law could be used to calculate ring-current strengths. I realized how stupid everybody had been because that is an obvious way to calculate them. Calculations of nucleus independent chemical shifts have been done since 1996 and noone realized that one should integrate NICS values. Luckily, we did not realize that 25 years ago because then GIMIC would not have been developed. More information than ring-current strengths are obtained with GIMIC. The magnetically induced current density (MICD) susceptibility is as fundamental for magnetic properties as the electron density is for molecular electrical properties. My coworkers and students have applied GIMIC to large interesting molecules. Mesias Orozco-Ic calculated the MICD for the figure-eight-shaped infinitene. We were fast an won the competition, the Salerno group lost and admitted it in the introduction of their paper. I liked that. Lukas Wirz is a wizard. I met him in New Zealand when he was PhD student in Peter Schwerdtfeger's group. He came to Helsinki as post-doc. Lukas masters graphs and their applications to carbon structures. He constructed the molecular structure of large Gaudiene-like molecules, all carbon toroids, . . . He made a knot of a carbon nanotorus.

Svenska Kemen, part 1

Svenska kemen existed for 50 years as a separate laboratory. Now, the scientfic personel is scattered around in the house. The rest of the staff were not replaced or moved to other laboratories. We had our coffee room were students could interact with the teachers. The threshold for asking questions was very low because they solved home exercises in our coffee room. I am able to identify the following persons in the photos. (from upper left) Susanne Lundberg, Henrik Konschin, Pekka Pyykkö, Bjarne Lindström, Henrik Tylli, Bertel Westermark, Michael Patzschke, Sebastian Hasenstab-Riedel, Dage Sundholm, Ville Kaila, Mikael Johansson, Gustav Boije, Juha Vaara, Mikaela Ekholm (and daughter), Jan Lundell, and Nino Runeberg. Many of the staff members and students became professors later. Sebastian Hasenstab-Riedel is professor at Freie Universität Berlin, Ville Kaila at Stockholm University, Juha Vaara at University of Oulu, Michael Patzschke at Helmholtz-Zentrum Dresden-Rossendorf, Jan Lundell at University of Helsinki (he moved recently from Jyväskylä University), Monika Österberg at Aalto University, Susanne Wiedmer at University of Helsinki, Nina Huittinen at Freie Universität Berlin. I might have forgotten somebody. However, we did something right.

Svenska Kemen, part 2

Before we moved to Kumpula, the laboratory was in the city center of Helsinki. The address was Etelä Hesperiankatu 4, near Finlandia hall. In the photo from Christmas 1992 we see: Bjarne Lindström, Jian Li, Henrik Tylli, Y. Zhao, Pekka Pyykkö, Bertel Westermark, Dage Sundholm, Mikaela Ekholm, Nino Runeberg, Monika Holmström (Österberg), and three more whose names I do not remember.

My Group in 2010

I became professor in 2010 and had a rather big research group. On the photo from left to right we see: Dage Sundholm, Krister Henriksson, Heike Fliegl, Stefan Taubert, Raul Mera, Sergio Losilla, Tommy Vänskä, Annika Tuomola, Michael Patzschke, Ville Kaila, Janne Pesonen, Olli Lehtonen, Cong Wang, Bertel Westermark, and Raija Eskelinen.

Computational Biochemistry, part 1

Henrik Konschin introduced computational biochemistry into the group. He had discussions with Mårten Wikström. Mårten did experimental studies on cytochrome C oxidase and realized in 1977 that it pumps protons across the membrane. Mårten debated with Peter Mitchell, who was awarded the Nobel Prize in chemistry in 1978. Peter admitted in the mid 1980:ies that he was wrong and Mårten was right. Henrik and Mårten convinced us to study computationally the oxygen reduction reaction of cytochrome C oxidase. Mårten covered the experimental aspects. Mikael Johansson was the PhD student that began with DFT calculations on this kind of biomolecules. Now, he does quantum computing at Centre for Scientific Computing. The very young Ville Kaila joined the project and took over and continues it today. Robert Send and Olli Lehtonen studied excitation processes of retinal and similar molecules. Robert Send works for an endoscopy company in Germany. Ville Kaila became full professor at the Technical University of Munich before he was 30 years old. He is now professor at Stockholm University.

Computational Biochemistry, part 2

Carl-Mikael Suomivuori was PhD student supervised by me and Ville. He is now professor at Yale School of Medicine. We studied photo-induced processes of biomolecules. We tackled questions like the color of wild lobsters and on the plate. We studied computationally the color of green fluorescent protein and how sodium is pumped across a membrane with the help of light.

Laxö a ”Tänkstäle”

The summer cottage at Laxö in Vexala is important for charging the battery. See the horizon, enjoy the sunset and swim whenever you want, if there is a hole in the ice.

Direct Approach to Gravitation and Electrostatics (2005-25), part 1

Now it was time for 3D. My idea for direct approach to gravitation and electrostatic (DAGE) came in 2001 or 2002. I presented it to Stefano Corni and Jeppe Olsen in 2002 when we discussed how to calculate properties of quantum dots. I implemented a test version and the first paper was published in 2005. Jonas Jusélius had implemented GIMIC and needed a new task. He did it properly and educated Sergio Losilla, who was an Erasmus student and became my PhD student. Sergio was very important for the project and for my group. He talked to students and was able to recruit talented students. Sergio implemented the bubble and cube algorithm, that is, a double grid method to treat the steep cusps of the electronic functions at the nuclei.

Direct Approach to Gravitation and Electrostatics (2005-25), part 2

The numerical team with Sergio as the experienced researcher and his students Elias Toivanen and Mooses Mehine did incredible things. Elias implemented a numerical fast multipole method. Mooses derived integral expression for seminumerical calculations of two- and three-electron integrals. I like the idea that cubes can be represented in spherical symmetry by using multipole moments. We talked about spherical boxes. Mooses was a better mathematician than the best students in mathematics, I was told. Unfortunately, neither Mooses nor Elias continued as PhD students.

Direct Approach to Gravitation and Electrostatics (2005-25), part 3

Wen-Hua Xu and Pauli Parkkinen were new postdocs. Eelis Solala was the new PhD student. Sergio left to the real world, which changed the character of the group. The social Spanish Sergio was replace by silent and bright Finns like Eelis and Pauli. Together with Wen-Hua Xu, they implemented the Helmholtz kernel for optimizing the orbitals and the generalized fast multipole moment method for optimizing orbitals. Finally we had a 3D code for numerical density functional theory calculations. Eelis implemented a numerical method for solving the response equations. The aim was to calculate polarizabilities and other second-order properties. Eelis worked on his PhD thesis and the last paper for the thesis when he got a flue that killed him, 29 years old. I felt very lonely. I finished Eelis thesis and printed 20 copies. I gave 10 copies to the family and kept 10 copies for myself and the group. Teemu Järvinen was the next researcher in the numerical group. He was sitting most of the time at home because of Covid-19. Last year I finished Eelis’ polarizability paper, I could touch his work again after 5 years.

Marathon (2004-11)

My old friends say that I am not only crazy, I am also stubborn. A nicer way to say it is that I have grit. I accepted a challenge almost 10 years ago. I promised to make 15000 pull ups in one year. Since then, I have made almost 180 000 pull ups. That is more than 50 pull ups every day during almost 10 years corresponding to more than 7 pull ups every day since I was born. I have survived 11 marathon runs. By best time is less than 4 hours. Grit is important. The first picture shows me when I approach the goal is my first marathon. The second picture is from my last Helsinki City Marathon. The last marathon was together with Jürgen Gauss in Frankfurt.

Photophysical Properties, part 1

Rashid Valiev was a young PhD student that came from Tomsk and wanted to work in my group. I realized that he is not an ordinary PhD student. We have studied computationally nonradiative processes of excited states. Our

first paper is from 2012 and now we have 48 common papers. Many of them are ”Hot Papers”. After a detour to Stockholm, he came back to Helsinki and will stay as long as he is employed. He does now computational atmospheric chemistry in Theo Kurtén's group. Rashid's contribution is calculations of photophysical properties of molecular systems of relevance in atmospheric chemistry. He develops methods to calculate rate constants for internal conversion of large molecules, which is very challenging. He recommended his PhD student Rinat Nasibullin as postdoc. Rinat is a programmer contributing to studies of photophysical properties. He has also contributed to the development and applications of GIMIC. He is now at Linköping University in Norrköping.

Photophysical Properties, part 2

One application of the methods to calculate nonradiative rate constants is computational studies of the optical yield of emitter molecules with temperature assisted delayed fluorescence (TADF) and 5^{th} generation emitter molecules, whose first excited state is a singlet. The TADF emitters are synthesized by researchers in Rioja. Daniel Blasco from University of La Rioja was postdoc in my group. He suggested a 5^{th} generation emitter molecule and synthesized it when he was back in Spain. It has an optical yield of fluorescence of 71% in solution and 33% in the solid state showing that also triplet excitons contributes to the fluorescence. He is now at Brno University of Technology. Our collaboration continues.

Spaniards and Latin Americans

I have had lots of research collaboration with researchers from Chile, Mexico and Spain. Fernando Mendizabal was postdoc here 30 years ago. The collaboration with us started and has continued since then. Researchers from Mexico also found us. Miguel Monge from Spain was guest researcher about 25 years ago. We have had research collaboration since then. Also his students have been here. Felix Reboiro from Rioja is now in Helsinki.

Alemanitos

When Fernando Mendizabal was in Helsinki, PhD students from Germany visited us. They came mainly from Hubert Schmidbauer's group. Fernando called them small Germans, that is Alemanitos. Since I have had active contacts with research groups in Germany, small Germans have visited and are still visiting the group. I hope the tradition continues, because German students are well educated. Raphael Berger was a small German before he came back to my group as postdoc. He is professor in Salzburg. The quality of the Alemanitos is very high. Yannick Franzke is today one of the main developers of Turbomole. Jonas Greiner belongs to the same group of excellent young scientists. I have many papers with Robert Send, who decided to go to industry later. Kevin Reiter and Mathias Pabst have also left the academia. Antonia Rabe is PhD student in Analytical Chemistry at Mainz university. Nina Winter, who contributed to the development of the ricc2 program, is head of the IT-service at University of Bochum.

Some Students

There is a number of PhD students that I might have not mentioned before. I hope that I have not forgotten anyone. Dou Du (China) got his PhD from Uppsala, he was my MSc student but could not get any funding for his PhD studies. After a post-doc at University of Lausanne, he is back in China. I have research collaboration with him. Failed applications are unfortunately a common denominator among PhD students. Lots of time is spent on writing applications instead of papers and theses. Hugo Åström is not my PhD student but we have a common paper and a common quantum computer project. The very international collection of PhD students are Isaac Benkyi (Ghana), Nergiz Özcan (Türkiye), Markus Rauhalahti (Finland), Qian Wang (China), Cong Wang (China), Atif Mahmood (Pakistan), Usman Ahmed (Pakistan), and Ying-Chan Lin (Taiwan).

Some Coworkers

Here, I mention some of the active coworkers and others that have been or are in Helsinki. Hassan Rabaâ (Morocco) is emeritus professor at University Ibn Tofail in Kenitra. He has regularly visited my group during the past 15 years. I have also visited Morocco several times. I have ongoing research collaboration with Martin Kaupp, who is professor at TU Berlin. Michael Patzschke came from Germany and became Pekka's PhD student, He worked may years here as university lecturer until he got a position in Dresden. Michal Straka was Pekka's PhD student. He is at Charles University in Prague. I have recently had research collaboration with him and and his student Lucie Tučková. Juha Vaara was researcher and university lecturer in Helsinki until he became professor in Oulu. Susi Lehtola has been many years in my group and many years researcher abroad. He is now Academy Researcher. I have had the pleasure to work with him. He is an excellent scientist with a huge international researcher network. He deserves a permanent position at University of Helsinki. He is also needed because the University of Helsinki cannot afford losing more theoretical chemistry. Developing quantum computing, machine learning and artificial intelligence for chemistry needs theory. These topics are in addition to the usual theory devlopment and know-how, which are needed to understand chemistry and chemical processes. Janne Pesonen is a mathematically oriented chemist. He writes a book about geometric algebra. Mathematically oriented chemists are not appreciated by chemists nor by mathematicians, because the chemists do not understand the mathematics and scientist have difficulties to accept researchers from other disciplines. I have ongoing research collaboration with Hiroshi Shinokubo from Nagoya University in Japan. He and his group synthesize novel porphyrinoids that we study computationally. I have ongoing research collaboration with Harapriya Rath at Indian Association for the Cultivation of Science, Kolkata, India. She and her group synthesize ferrocene containing porphyrinoids, which we study computationally. Susanne Wiedmer was university lecturer and is now professor of Analytical Chemistry at the University of Helsinki. Yavus Dede from Gazi University in Ankara was recently guest professor in my group.

Before Ending, part 1

Today, I have presented my scientific Curriculum Vitae. I have discussed research directions and the role of some of my coworkers. It is impossible to review everything in one lecture, since I have published more than 330 scientific papers and a few book chapters. I have presented my main research directions and discussed my way of thinking. Planning research is not my piece of cake. My research directions are to some extent constructions afterwards. Decisions were made and I did not always know why. I followed my intuition. The dice are rolled and the consequences were taken. Many ingredients are needed to make a successful researcher: Education, creativity, skill, talent, intuition, luck, grit and coworkers. The Academy of Finland (The Research Council of Finland) has supported me from the beginning to the last year. EU supported me 20 years ago, before the projects became incredible big and expensive. I applied for ERC grants a few times, in vain. University of Helsinki has been less generous. It has paid my salary, given us office space. Four-five times I received smaller amount of research funding. University of Helsinki even took once my external funding because it had been on the account too long. Funding from private foundations has been crucial as well as research visitors with own funding. In house research collaboration is good but external research collaboration is better because you can choose the coworkers and not marry your cousin.

Before Ending, part 2

Helsingin Yliopistokiinteistöt Oy is a University of Helsinki owned company that owns for example this building, Its turnover in 2024 was 68.0 M€ consisting entirely of rental income. It was an increase of 6.4% from 2023. The company's result was 22.2 M€. Why must a university owned company make profit when the income is from internal sources? Finland introduced the JUFO system, which means that every scientific article brings funding to the university, which is never seen in the funding of the research group publishing the scientific articles. If the research groups could keep a significant part of the JUFO funding, PhD students could contribute to their own salary by writing scientific articles instead of in many cases unsuccessful applications to private foundations. I showed pictures of Svenska Kemen, which was an active laboratory educating students and doing research. Many future professors were educated there. The staff was shrinking during my time as professor and distributed to other units at the Department of Chemistry. The reason was not bad performance but other units at the department needed

the resources. My retirement was also the end of the professorship in theoretical chemistry at the University of Helsinki, not because of bad performance but because the resources were allocated for other activities.

The End

I have always been a small boy supporting the weak. I would like to thank all coworkers, without their efforts I would have had much less to talk about today. I have had young coworkers who during the projects turned into skillful researchers and it happens remarkably fast. Chemists must allow themselves to do research in areas that do not lead to a product in the foreseeable future. That research can contribute to future technology and pushes the boundaries of our knowledge.

Eliel Saarinen was a Finnish and American architect, designer, and urban planner. The Finnish pavilion at the Paris 1900 World Fair was his first major work with Gesellius and Lindgren. They built the Hvitträsk mansion complex in Kirkkonummi about 30 km west of Helsinki. It was designed as a studio home by Gesellius, Lindgren, Saarinen and become later the private residence of Eliel Saarinen. It is now a museum that is worth a visit. You find his headstone there.

I end here by citing the last statement (number 7) in Tractatus Logico-Philosophicus by Ludwig Wittgenstein. ”Wovon man nicht sprechen kann, darüber muss man schweigen”. (Whereof one cannot speak, thereof one must be silent.)