FAREWELL LECTURE

Professor emeritus Dage Sundholm

Department of Chemistry,
University of Helsinki

May 4, 2026

CHILDHOOD

Summer 1958

May 1964

I was born on December 22, 1957

My father Karl was a fisherman until 1959

He started with my mother Terese 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 also became a strong boy as mink farmer

The small and youngest boy was arm wrestling master

Childhood home (picture from 1997)

Fishing baltic herring

Dage and Jan in 1964

School

Vexala public school in May 1965

Seven classes and six pupils per class

Two teachers and a cook

I began in the fall 1964, but 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

In 1968, the school was closed

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 (Topelius Gymnasium)

I got my high-school diploma in 1976

University studies

University studies were rare among young people in Vexala. 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 working in IT.

Karl-Gustav Fogel, Professor of Physics and Rector of the Åbo Akademi Unversity was born in Vexala and had his summer place near my childhood home. He was my father's second cousin.

Kurt Nyholm, Professor of Germanic Philology and Rector of the Åbo Akademi Unversity 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, I decided to take more courses than the obligatory ones. After four years, I had taken almost all courses that were available (except some central courses in process engineering).

UNIVERSITY STUDIES

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*"

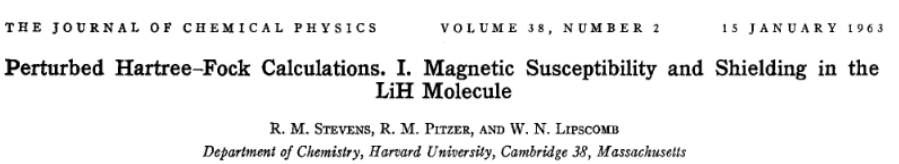
I was interested in PhD studies and asked Professor Lindfors whether he had funding for a PhD student. The answer was no. I then asked Professor Pekka Pyykkö. His answer was yes.

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 Nordic Conference on Surface Science, Tampere, 1982 (no paper)

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 this article, which is relevant for my recent research (spatial contributions to NMR chemical shifts)



THE JOURNAL OF CHEMICAL PHYSICS VOLUME 38, NUMBER 2 15 JANUARY 1963

Perturbed Hartree–Fock Calculations. I. Magnetic Susceptibility and Shielding in the LiH Molecule

R. M. STEVENS, R. M. PITZER, AND W. N. LIPSCOMB
Department of Chemistry, Harvard University, Cambridge 38, Massachusetts
(Received 10 September 1962)

Entering the quantum chemistry community at Åbo Akademi

Participating in the International Congress of Quantum Chemistry (ICQC) 1982 in Uppsala
Matti Hotokka, me and Leif Laaksonen

(Upper picture) from left to right: me, Matti Hotokka, Arlen Viste, Pekka Pyykkö, Jean-Paul Desclaux, Leif Laaksonen

Relativistic Effects in Quantum Chemistry, in Åbo
A satellite conference to ICQC 1982

MOVING TO HELSINKI

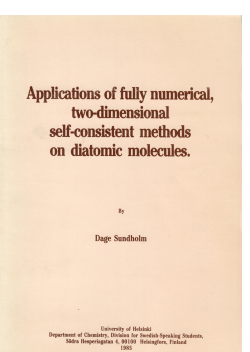
The numercial project was in close collaboration with Leif Laaksonen, who defended his thesis "*Two-dimensional fully numerical solutions of molecular Schrödinger equations*" at Åbo Akademi University in 1983.

The title of my Licentiate of Technology thesis was "*Tvådimensionella Numeriska Lösningar till Molekylära Hartree-Fock och Hartree-Fock-Slater Ekvationer*", Åbo Akademi University, 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 PhD was not the end, it was the end of the beginning (Winston Churchill)

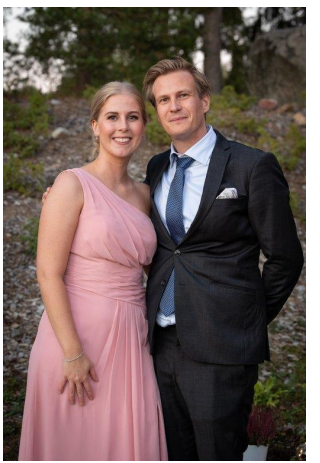


Jean-Paul Desclaux, Pekka Pyykkö, and Dage Sundholm

THE FAMILY

In 1986
Maj-Len, Dage

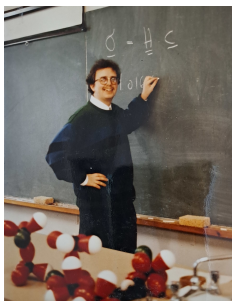
In 2019
Dage, Maj-Len, Johnny, Merve, Mathias



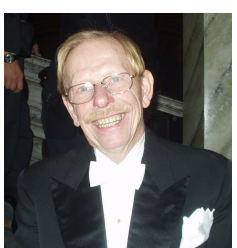
In 2024
Charlotta, Johnny

In 2025
Merve, Aylin, Mathias

LUND UNIVERSITY (1986-88)



Jeppe Olsen



Björn Roos

Converting from finite differences to finite elements

A BLOCK PRECONDITIONED CONJUGATE GRADIENT METHOD FOR SOLVING HIGH-ORDER FINITE ELEMENT MATRIX EQUATIONS

Computer Physics Communications 49 (1988) 409–415

Dage SUNDHOLM *

Theoretical Chemistry, Chemical Centre, University of Lund, Box 124, S-221 00 Lund, Sweden

NUMERICAL MCSCF IN ONE AND TWO DIMENSIONS

Dage Sundholm, Jeppe Olsen, Per-Åke Malmqvist and Björn O. Roos
Theoretical Chemistry, Chemical Center
P.O.B. 124, S-221 00 LUND, Sweden

Proceedings of NATO Advanced Research Workshop, Versailles 1988

Changing from 2D to 1D

Large multiconfigurational Hartree-Fock calculations on the hyperfine structure of Li(^2S) and Li(^2P)

Dage Sundholm
Department of Chemistry, University of Helsinki, Et. Hesperiank. 4, SF-00100 Helsinki, Finland

Jeppe Olsen
Theoretical Chemistry, Chemical Centre, University of Lund, P.O. Box 124, S-22100 Lund, Sweden
(Received 15 February 1990; revised manuscript received 10 April 1990)

Phys. Rev. A 42 (1990) 2614-2621 was the first of a series of 25 articles.

However, atomic physics had no future in the 1990:ies, nanotechnology came

It was time to move on.

UNIVERSITY OF HELSINKI (1988-1993)

I had a Laboratory instructor position as background job (1986-1995)

I was on leave most of the time (when I was in Lund).

My PhD studies were supported by Pekka's AKA project

I had positions at the Academy of Finland (1990-1991 and 1992-1997)

My salary was mainly paid from AKA grants in 1981-1985, AKA research positions in 1990-1997, and AKA grants in 1999-2010.

I have had continuous AKA projects (2002-2025).

I was twice in the final for Academy Professor positions

The Academy of Finland (AKA) 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.

Maria Göppert-Mayer developed the theory in her PhD thesis in 1930.

They were developing a computational method to calculate two-photon absorption spectra.

The theoretical spectroscopy expert Antonio Rizzo (CNR, Pisa) also visited Århus

Multiconfiguration self-consistent field quadratic response calculations of the two-photon transition probability rate constants for argon

Dage Sundholm
Department of Chemistry, P.O. Box 19 (Et. Hesperiank. 4), FIN-00014 University of Helsinki, Finland
Antonio Rizzo
Istituto di Chimica Quantistica ed Energetica Molecolare del CNR, Via Risorgimento 35, I-56100 Pisa, Italy
Poul Jørgensen
Department of Chemistry, Aarhus University, DK-8000 Aarhus C, Denmark

J. Chem. Phys. 101 (1994) 4931-4935.

The two-photon absorption spectrum of CO was also studied.

Poul Jørgensen

Antonio Rizzo

Århus was the first stop on our way to Karlsruhe

University of Karlsruhe (1994-1995)

Reinhart Ahlrichs

Jürgen Gauss

The Turbomole program was developed in Karlsruhe

Marco Häser developed the direct SCF program
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

Ansgar Schäfer was doctoral student developing basis sets

Christian Ochsenfeld was doctoral student performing calculations on salt (Na_nCl_n)

There were many other young researchers in the Ahlrichs group

Christian Ochsenfeld

Ansgar Schäfer

UNIVERSITY OF KARLSRUHE (1994-1995)

The electron correlation contribution to the nuclear magnetic shielding tensor of the hydrogen molecule

Dage Sundholm [1], Jürgen Gauss, Reinhart Ahlrichs

Chemical Physics Letters 243 (1995) 264–268

J. Am. Chem. Soc. **1995,** *117,* 11523−11528 11523

Ab Initio Study of Nuclear Magnetic Shieldings and Ultraviolet Spectra for Hypothiocyanite and Its Isomers. The Molecular Structure of Hypothiocyanite

Dage Sundholm†

Contribution from the Institut für Physikalische Chemie, Lehrstuhl für Theoretische Chemie, Universität Karlsruhe, D-76128 Karlsruhe, Germany

J. Chem. Phys. **105** (24), 22 December 1996

Rovibrationally averaged nuclear magnetic shielding tensors calculated at the coupled-cluster level

Dage Sundholm
Department of Chemistry, University of Helsinki, P.O. Box 55 (A.I. Virtasen aukio 1), FIN-00014 Helsinki, Finland

Jürgen Gauss
Institut für Physikalische Chemie, Universität Mainz, D-55099 Mainz, Germany

Ansgar Schäfer[a)]
Lehrstuhl für Theoretische Chemie, Institut für Physikalische Chemie, Universität Karlsruhe, D-76128 Karlsruhe, Germany

Chem. Eur. J. **1999**, *5*, 267

An Ab Initio Study of Structure and Energetics of Free-Base Bonellin-Dimethylester Isomers and Transition States

Dage Sundholm,*[a] Henrik Konschin,[a] and Marco Häser[b]

Good friends

Skat (Nachtisch)

Magnetic properties

Large molecules

Rock climbing (Pfalz and Schwarzwald)

Mountaineering

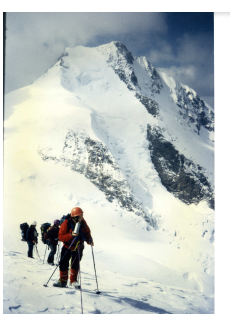
- Ofenhorn (3235 m)
- Bellavista (3921 m) (Bernina)
- Hiking in Utah

BERNINA TOUR

Ascent towards Marco e Rosa

Climbing along Bellavista

Leaving Marco e Rosa



Bernina in the background

Marco Häser smiling in the Diavolezza hut

I am not smiling in the Diavolezza hut

Mount Timpanogous tour (3582 m)

Hiking with Christian Ochsenfeld and Maj-Len in Utah 1996

QUANTUM DOTS (1999-2003)

L REVIEW B VOLUME 61, 7652

Full configuration interaction calculations of electron-hole correlation effects in strain-induced quantum dots

M. Braskén and M. Lindberg
Department of Physics, Åbo Akademi University, FIN-20500 Turku, Finland

D. Sundholm
Department of Chemistry, University of Helsinki, FIN-00014 Helsinki, Finland

J. Olsen
Department of Chemistry, University of Aarhus, DK-8000 Aarhus, Denmark

Mats Braskén

Markus Lindberg

PHYSICAL REVIEW B **67**, 085314 (2003)

Electron-hole recombination density matrices obtained from large configuration-interaction expansions

S. Corni
Scuola Normale Superiore, Piazza dei Cavalieri 7, I-56126 Pisa, Italy

M. Braskén
Swedish Polytechnic, Finland, FIN-65200 Vaasa, Finland

M. Lindberg
Department of Physics, Åbo Akademi University, FIN-20500 Turku, Finland

J. Olsen
Department of Chemistry, University of Aarhus, DK-8000 Aarhus, Denmark

D. Sundholm
Department of Chemistry, University of Helsinki, FIN-00014 Helsinki, Finland

Stefano Corni

Jeppe Olsen

JUST FOR FUN

Tommy Vänskä

Markus Lindberg

Perturbation energy expansions based on two-component relativistic Hamiltonians

Dage Sundholm

Theor Chem Acc (2003) 110: 144–152
DOI 10.1007/s00214-003-0465-z

A configuration interaction approach to bosonic systems

J. Phys. B: At. Mol. Opt. Phys. **37** (2004) 2933–2942

D Sundholm and T Vänskä

PHYSICAL REVIEW A **75**, 023621 (2007)

Configuration-interaction studies of Bose-Einstein condensates

T. Vänskä and D. Sundholm
Department of Chemistry, P.O. Box 55 (A.I. Virtasen aukio 1), FIN-00014 University of Helsinki, Finland

M. Lindberg
Department of Physics, Åbo Akademi University, Porthansgatan 3, FIN-20500 Turku, Finland
(Received 5 October 2006; published 26 February 2007)

THE JOURNAL OF CHEMICAL PHYSICS **140**, 234111 (2014)

On energetic prerequisites of attracting electrons

Dage Sundholm
Department of Chemistry, POB 55 (A.I. Virtanens plats 1), FIN-00014 University of Helsinki, Finland

Don't be too analytical

Design an approproiate local relation between the small and the large component

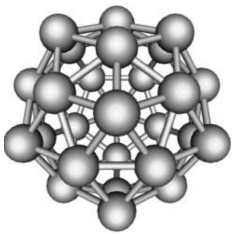
Relativistic perturbation theory based on quasi-relativistic Hamiltonians

Numbering of boson configurations using orbital indices

We wrote a CI program for bosons

Be brave, new ideas are always needed but not necessarily always appreciated

JUST FOR FUN

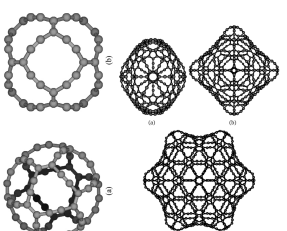


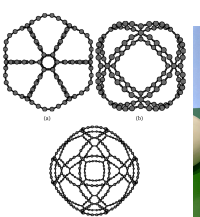
Au_{32}: A 24-Carat Golden Fullerene**

Angew. Chem. Int. Ed. **2004**, *43*, 2678 –2681

Mikael P. Johansson, Dage Sundholm, and Juha Vaara*

Au_{32} was constructed from fullerene. Each face center was replaced by Au and all C atoms were removed.





C_{72}: gaudiene, a hollow and aromatic all-carbon molecule†

Cite this: *Phys. Chem. Chem. Phys.*, 2013, **15**, 9025

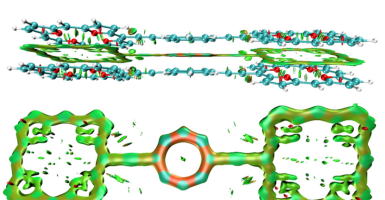
Dage Sundholm*

Novel hollow all-carbon structures†

Cite this: *Nanoscale*, 2015, **7**, 15886

Dage Sundholm,*[a] Lukas N. Wirz[b] and Peter Schwerdtfeger*[c]

The photo in Sagrada Familia showed an all-carbon structure, I called it Gaudiene



Change of the aromatic nature through face-to-face stacking†

Qian Wang,[a‡] Rinat T. Nasibullin,[a‡] and Dage Sundholm[a]

Aromatic bonding of antiaromatic molecules, a new kind of chemical bond

WINTER SCHOOL IN THEORETICAL CHEMISTRY (1985-)

Pekka Pyykkö started the Winter School series in 1985

I got organization responsibilities in the late 1990ies and in 2000 to 2009, I had the main responsibility

1985 Applied Quantum Chemistry
1986 Liquid Crystals
1987 Quantum Chemistry
1988 Molecular Dynamics and Quantum Pharmacology
1989 New Chemical Species and Their Detection
1990 DNA, Heavy Metals and their Interactions
1991 Quantum Chemistry of Complex Systems
1992 Condensed Matter: From Metals to Membranes
1993 Colloid Chemistry in Materials Science
1994 Relativity and Pseudopotentials
1995 Calculation of NMR Parameters
1996 Determination of Nuclear Quadrupole Moments
1997 Solvation
1998 Chemical Reactions
1999 Electron and Proton Transfer in Biological Systems
2000 Magnetic Properties of Molecules
2001 Condensed Phase Dynamics
2002 Large Molecules: Linear Scaling and Related Electronic Structure Calculation Methods
2003 Quantum Chemistry Bordering Nanoscience and Nanotechnology
2004 A Frontier of Chemistry: New Species

WINTER SCHOOL IN THEORETICAL CHEMISTRY (1985-)

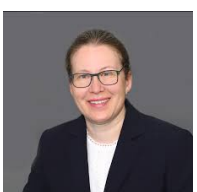
I have been the main organizer during the past 15 years.

My older colleagues have later taken more responsibility and students have helped

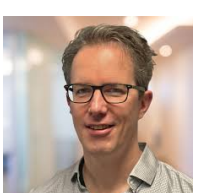
2005 Nanophotonics
2006 Astrochemistry
2007 Actinide Chemistry
2008 Reactions on Surfaces - Towards Realistic Computational Modelling of Surface Reactions
2009 Chemical Bonding
2010 Accurate Molecular Structure by Experiment and Theory
2011 Excited State Properties
2012 Nuclear motion in molecules
2013 Theoretical Spectroscopy
2014 Theoretical f-Element Chemistry
2015 Computational Biohemistry
2016 Current Trends in Electronic Structure Theory Methods
2017 Molecular Energy and Electron Transfer
2018 Machine Learning in Theoretical Chemistry
2019 Inorganic Chemistry
2020-2021 Cancelled
2022 QC-4C: Quantum Computers for Chemistry
2023 Dynamic processes of molecules in electronic excited state
2024 Solvation and Embedding
2025 Electronic Structure Theory

MAGNETICALLY INDUCED CURRENT DENSITY SUSCEPTIBILITY (GIMIC) (2004-)

Jonas Jusélius



Heike Fliegl



Radovan Bast

JOURNAL OF CHEMICAL PHYSICS VOLUME 121, 3952

Calculation of current densities using gauge-including atomic orbitals

Jonas Jusélius and Dage Sundholm[a)]
Department of Chemistry, P.O. Box 55 (A.I. Virtasen Aukio 1), FIN-00014 University of Helsinki, Helsinki, Finland
Jürgen Gauss[b)]
Institut für Physikalische Chemie, Universität Mainz, Jakob-Welder Weg 11, D-55099 Mainz, Germany

THE JOURNAL OF CHEMICAL PHYSICS **134**, 054123 (2011)

Calculation of spin-current densities using gauge-including atomic orbitals

StefanTaubert,[1,a)] Dage Sundholm,[1,b)] and Jonas Jusélius[2,c)]
[1]*Department of Chemistry, P.O. Box 55 (A.I. Virtanens plats 1), University of Helsinki, FIN-00014 Finland*
[2]*Department of Chemistry, University of Tromsø, N-9037 Tromsø, Norway*

Spatial Contributions to Nuclear Magnetic Shieldings

Published as part of The Journal of Physical Chemistry virtual special issue "Alexander Boldyrev Festschrift".

Rahul Kumar Jinger, Heike Fliegl, Radovan Bast, Maria Dimitrova, Susi Lehtola, and Dage Sundholm*

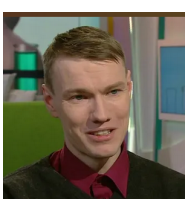
Cite This: *J. Phys. Chem. A* 2021, 125, 1778−1786 Read Online

Check for updates
Cite this: *Chem. Sci.*, 2025, **16**, 8040
All publication charges for this article have been paid for by the Royal Society of Chemistry

Orbital contributions to magnetically induced current densities using gauge-including atomic orbitals†

Rinat T. Nasibullin,* Maria Dimitrova, Rashid R. Valiev and Dage Sundholm *

Jürgen Gauss



Stefan Taubert

Rinat Nasibullin

GIMIC Review and book chapters

Vincent Liégeois

Maria Dimitrova

Raphael Berger

Calculations of magnetically induced current densities: theory and applications

Dage Sundholm,[1]* Heike Fliegl[2] and Raphael J.F. Berger[3]

WIREs Comput Mol Sci 2016, 6:639–678.

CHAPTER 5

Magnetically Induced Current Densities and Nuclear Magnetic Shielding Constants

D. SUNDHOLM,* M. DIMITROVA AND D. BLASCO

Department of Chemistry, University of Helsinki, P.O. Box 55 (A.I. Virtanens Plats 1), FIN-00014, Finland
*Email: sundholm@chem.helsinki.fi

Series New Developments in NMR, NMR Spectroscopic Parameters: Theories and Models, Computational Codes and Calculations ", Ed. G. A. Aucar, 2025 eBook Collection Royal Society of Chemistry 38 (2025) 170-204.

218 Aromatic Pathways in Porphyrinoids by Magnetically Induced Ring Currents

Dage Sundholm* and Heike Fliegl†

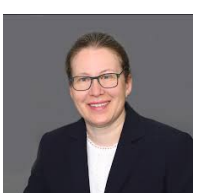
Chapter 218 in Handbook of Porphyrin Science, Vol. 46, Eds K. M. Kadish, K. M. Smith and R. Guilard, World Scientific (2022)

Current density, current-density pathways and molecular aromaticity

Maria Dimitrova and Dage Sundholm

Chapter 5 in Aromaticity: Modern Computational Methods and Applications, Ed. I. Fernández López, Elsevier (2021) pp. 155-194

Daniel Blasco



Heike Fliegl

SELECTION OF RECENT GIMIC APPLICATIONS

Maria Dimitrova

Rashid Valiev

Lukas Wirz

Check for updates

Cite this: *Phys. Chem. Chem. Phys.*, 2022, **24**, 624

Received 5th November 2021,
Accepted 10th December 2021

Integration of global ring currents using the Ampère–Maxwell law†

Raphael J. F. Berger, [a*] Maria Dimitrova, [ab] Rinat T. Nasibullin, [c] Rashid R. Valiev [bc] and Dage Sundholm [b*]

Check for updates

Cite this: *Phys. Chem. Chem. Phys.*, 2022, **24**, 1666

Magnetically induced ring currents in metallocenothiaporphyrins†

Rashid R. Valiev, [ab] Theo Kurten, [b] Lenara I. Valiulina, [a] Sergey Yu. Ketkov, [c] Viktor N. Cherepanov, [a] Maria Dimitrova [b] and Dage Sundholm [b*]

Check for updates

Cite this: *Phys. Chem. Chem. Phys.*, 2022, **24**, 6404

Non-intersecting ring currents in [12]infinitene†

Mesías Orozco-Ic, [a*] Rashid R. Valiev [ab] and Dage Sundholm [a*]

Check for updates

Cite this: *Phys. Chem. Chem. Phys.*, 2023, **25**, 12469

Current-density pathways in figure-eight-shaped octaphyrins†

Qian Wang, Jaakko Pyykkö, Maria Dimitrova, Stefan Taubert and Dage Sundholm *

Check for updates

Cite this: *Phys. Chem. Chem. Phys.*, 2024, **26**, 14777

Changing aromatic properties through stacking: the face-to-face dimer of Ni(II) bis(pentafluorophenyl)norcorrole†

Qian Wang, [a] Dage Sundholm, [a*] Jürgen Gauss, [b] Tommaso Nottoli, [c] Filippo Lipparini, [c] Shota Kino, [d] Shusaku Ukai, [d] Norihito Fukui [de] and Hiroshi Shinokubo [d]

Magnetically Induced Current Densities in Toroidal Carbon Nanotubes

J. Phys. Chem. C 2019, 123, 15354−15365

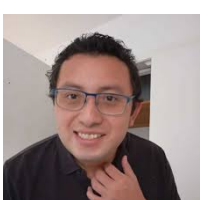
Kevin Reiter, [†,§] Florian Weigend, [†] Lukas N. Wirz, [*,†,‡] Maria Dimitrova, [‡] and Dage Sundholm [*,‡]

[†]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen, Germany

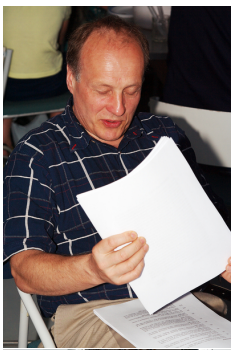
[‡]Department of Chemistry, University of Helsinki, P.O. Box 55, A. I. Virtasen Aukio 1, FIN-00014 Helsinki, Finland

Raphael Berger

Qian Wang Jaakko Paaer



Mesías Orozco-Ic



Susanne Lundberg, Henrik Konschin, Pekka Pyykkö, Bjarne Lindström, Henrik Tylli, Bertel Westermark, Michael Patzschke, Sebastian Riedel, Dage Sundholm, Ville Kaila, Mikael Johansson, Gustav Boije, Juha Vaara, Mikaela Ekholm (and daughter), Jan Lundell, Nino Runeberg

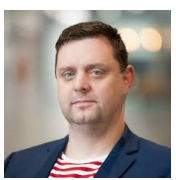
Christmas 1992 Bjarne Lindström, Jian Li, Henrik Tylli, Y. Zhao, Pekka Pyykkö, Bertel Westermark, Dage Sundholm, Mikaela Ekholm, Nino Runeberg, Monika Holmström (Österberg), and three more that I do not remember

My group in 2010

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, Raija Eskelinen

COMPUTATIONAL BIOCHEMISTRY (2002-2020)

Ville Kaila



Mikael Johansson

Robert Send

J. AM. CHEM. SOC. 2002, *124*, 11771−11780

The Spin Distribution in Low-Spin Iron Porphyrins

Mikael P. Johansson,*,† Dage Sundholm,†,|| Gary Gerfen,‡,⊥ and Mårten Wikström§,#

Contribution from the Department of Chemistry, P.O. Box 55 FIN-00014, University of Helsinki, Finland, Department of Physiology and Biophysics, Albert Einstein College of Medicine, 1300 Morris Park Avenue, Bronx, New York 10461, and Helsinki Bioenergetics Group, Institute of Biotechnology, P.O. Box 65 FIN-00014 University of Helsinki, Finland

THE JOURNAL OF CHEMICAL PHYSICS **131**, 024301 (2009)

Coupled-cluster and density functional theory studies of the electronic excitation spectra of *trans*-1,3-butadiene and *trans*-2-propeniminium

Olli Lehtonen,[1,a)] Dage Sundholm,[1] Robert Send,[2] and Mikael P. Johansson[3]
[1]*Department of Chemistry, University of Helsinki, POB 55 (A.I. Virtanens plats 1), Helsinki FIN-00014, Finland*
[2]*Institut für Physikalische Chemie, Universität Karlsruhe, Kaiserstrasse 12, 76128 Karlsruhe, Germany*
[3]*Lundbeck Foundation Center for Theoretical Chemistry, Aarhus University, Langelandsgade 140, DK-8000 Århus C, Denmark*

21470–21475 | PNAS | December 14, 2010 | vol. 107

Interheme electron tunneling in cytochrome *c* oxidase

Ville R. I. Kaila[a,b,1,2], Mikael P. Johansson[b,c,1], Dage Sundholm[b], and Mårten Wikström[a,1]

[a]Helsinki Bioenergetics Group, Structural Biology and Biophysics Programme, Institute of Biotechnology, University of Helsinki, P.O. Box 65, FI-00014 Helsinki, Finland; [b]Department of Chemistry, University of Helsinki, P.O. Box 55, FI-00014 Helsinki, Finland; and [c]Institut de Quimica Computacional, Universitat de Girona, Campus Montilivi, 17071 Girona, Spain

J. Phys. Chem. B 2012, 116, 2249–2258

The Effect of Protein Environment on Photoexcitation Properties of Retinal

Ville R. I. Kaila,*,† Robert Send,*,‡ and Dage Sundholm*,§

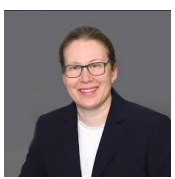
Mårten Wikström

Henrik Konschin

Olli Lehtonen

COMPUTATIONAL BIOCHEMISTRY (2002-2020)

Ville Kaila



Heike Fliegl

Robert Send

J. Phys. Chem. B 2015, 119, 2933−2945

Coupled-Cluster Studies of Extensive Green Fluorescent Protein Models Using the Reduced Virtual Space Approach

Robert Send,[*,†,∥] Carl-Mikael Suomivuori,[‡,∥] Ville R. I. Kaila,[*,§] and Dage Sundholm[*,‡]

[†]BASF SE, Quantum Chemistry Group, GVM/M - B009, D-67056 Ludwigshafen, Germany
[‡]Department of Chemistry, University of Helsinki, P.O. Box 55 (A. I. Virtanens plats 1), FI-00014 Helsinki, Finland
[§]Department Chemie, Technische Universität München, Lichtenbergstraße 4, D-85747 Garching, Munich, Germany

Angew. Chem. Int. Ed. 2015, 54, 11564 –11566

Protein-Induced Color Shift of Carotenoids in β-Crustacyanin**

*Ana P. Gamiz-Hernandez, Iva Neycheva Angelova, Robert Send, Dage Sundholm, and Ville R. I. Kaila**

PNAS | July 3, 2017 | vol. 114 | no. 27 | 7043–7048

Energetics and dynamics of a light-driven sodium-pumping rhodopsin

Carl-Mikael Suomivuori[a,b], Ana P. Gamiz-Hernandez[b], Dage Sundholm[a], and Ville R. I. Kaila[b,1]

[a]Department of Chemistry, University of Helsinki, FIN-00014 Helsinki, Finland; and [b]Department Chemie, Technische Universität München, D-85747 Garching, Germany

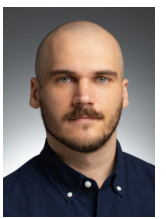
Check for updates

Cite this: Phys. Chem. Chem. Phys., 2019, 21, 6851

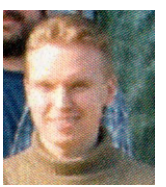
Absorption shifts of diastereotopically ligated chlorophyll dimers of photosystem I†

Carl-Mikael Suomivuori, [a] Heike Fliegl, [b] Evgeni B. Starikov, [c] T. Silviu Balaban,[‡] Ville R. I. Kaila [e] and Dage Sundholm [*,†]

Mårten Wikström



Carl-Mikael Suomivuori

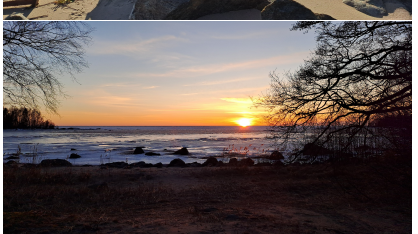
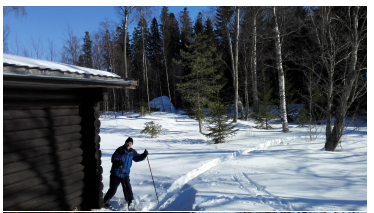


Olli Lehtonen

LAXÖ A ”TÄNKSTÄLLE”





DIRECT APPROACH TO GRAVITATION AND ELECTROSTATICS (2005-2025)

Jonas Jusélius

Sergio Losilla

The numerical team

Finite-element methods for 3D numerical calculations of molecular electronic structure

Wen-Hua Xu

Pauli Parkkinen

THE JOURNAL OF CHEMICAL PHYSICS **122**, 194107 (2005)

Universal method for computation of electrostatic potentials

D. Sundholm
Department of Chemistry, University of Helsinki, FIN-00014 Helsinki, Finland

Elias Toivanen

THE JOURNAL OF CHEMICAL PHYSICS **132**, 024102 (2010)

The direct approach to gravitation and electrostatics method for periodic systems

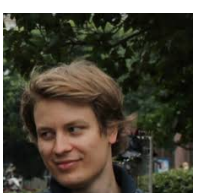
S. A. Losilla,[1] D. Sundholm,[1,a)] and J. Jusélius[2]
[1]*Department of Chemistry, University of Helsinki, FIN-00014 Helsinki, Finland*
[2]*Department of Chemistry, University of Tromsø, N-9037 Tromsø, Norway*

Eelis Solala

THE JOURNAL OF CHEMICAL PHYSICS **136**, 214104 (2012)

A divide and conquer real-space approach for all-electron molecular electrostatic potentials and interaction energies

S. A. Losilla and D. Sundholm
Department of Chemistry, University of Helsinki, FIN-00014 Helsinki, Finland



Mooses Mehine

DIRECT APPROACH TO GRAVITATION AND ELECTROSTATICS (2005-2025)

Sergio Losilla

Wen-Hua Xu

Eelis Solala

Molecular Physics
Vol. 110, Nos. 19–20, October 2012, 2569–2578

Construction of the two-electron contribution to the Fock matrix by numerical integration

Sergio A. Losilla*, Mooses M. Mehine and Dage Sundholm

Department of Chemistry, University of Helsinki, A.I. Virtanens plats 1, FIN-00014 Helsinki, Finland

Molecular Physics, 2013
Vol. 111, Nos. 16–17, 2536–2543

An efficient algorithm to calculate three-electron integrals for Gaussian-type orbitals using numerical integration

Mooses M. Mehine, Sergio A. Losilla and Dage Sundholm*

Department of Chemistry, University of Helsinki, Helsinki, Finland

Construction of the Fock Matrix on a Grid-Based Molecular Orbital Basis Using GPGPUs

DOI: 10.1021/ct501128u
J. Chem. Theory Comput. 2015, 11, 2053−2062

Sergio A. Losilla,[†,||] Mark A. Watson,[‡] Alán Aspuru-Guzik,[§] and Dage Sundholm*[,†]

[†]Department of Chemistry, University of Helsinki, P.O. Box 55, FIN-00014 Helsinki, Finland
[‡]Schrödinger, Inc, 120 West 45th Street, New York, New York 10036, United States
[§]Department of Chemistry and Chemical Biology, Harvard University, Cambridge, Massachusetts 02138, United States

CrossMark click for updates

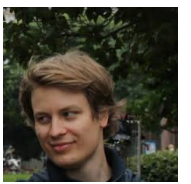
Cite this: *Phys. Chem. Chem. Phys.*, 2015, **17**, 31480

The grid-based fast multipole method – a massively parallel numerical scheme for calculating two-electron interaction energies

Elias A. Toivanen, Sergio A. Losilla† and Dage Sundholm*

Pauli Parkkinen

Elias Toivanen



Mooses Mehine

DIRECT APPROACH TO GRAVITATION AND ELECTROSTATICS (2005-2025)

Sergio Losilla

Wen-Hua Xu

Eelis Solala

THE JOURNAL OF CHEMICAL PHYSICS **146**, 084102 (2017)

Optimization of numerical orbitals using the Helmholtz kernel

Eelis Solala, Sergio A. Losilla, Dage Sundholm, Wenhua Xu, and Pauli Parkkinen
Department of Chemistry, University of Helsinki, P.O. Box 55, A.I. Virtanens plats 1, FIN-00014 Helsinki, Finland

A Generalized Grid-Based Fast Multipole Method for Integrating Helmholtz Kernels

DOI: 10.1021/acs.jctc.6b01207
J. Chem. Theory Comput. 2017, 13, 654−665

Pauli Parkkinen, Sergio A. Losilla, Eelis Solala, Elias A. Toivanen, Wen-Hua Xu,[†] and Dage Sundholm*

Department of Chemistry, University of Helsinki, P.O. Box 55, A. I. Virtanens plats 1, Helsinki FIN-00014, Finland

Density Functional Theory under the Bubbles and Cube Numerical Framework

J. Chem. Theory Comput. 2018, 14, 4237−4245

Pauli Parkkinen,[†] Wen-Hua Xu,[†,‡] Eelis Solala,[†] and Dage Sundholm*,[†,§]

[†]Department of Chemistry, University of Helsinki, P.O. Box 55 (A. I. Virtanens plats 1), FIN-00014 Helsinki, Finland
[‡]College of Chemistry and Materials Science, Northwest University, Xi'an 710069, China
[§]Centre for Advanced Study at the Norwegian Academy of Science and Letters, Drammensveien 78, N-0271 Oslo, Norway

Numerical Calculations of Electric Response Properties Using the Bubbles and Cube Framework

J. Phys. Chem. A 2025, 129, 3368−3374

Published as part of The Journal of Physical Chemistry A special issue "Forty Years of Response Function Theory".

Eelis Solala, Wen-Hua Xu, Pauli Parkkinen, and Dage Sundholm*

Pauli Parkkinen

Elias Toivanen

Teemu Järvinen

MARATHON (2004-2011)

Almost 180000 pull ups since 12.9.2016

on the average more than 50 pull ups every day since then

More than 7 every day since I was born

Survived 11 Marathon runs
(best time 3:53:23)

It is never too late to give up

Grit is important

PHOTOPHYSICAL PROPERTIES (2012-)

Rashid Valiev

Check for updates

Cite this: *Phys. Chem. Chem. Phys.*, 2018, **20**, 6121

First-principles method for calculating the rate constants of internal-conversion and intersystem-crossing transitions†

R. R. Valiev,[a*b] V. N. Cherepanov,[a] G. V. Baryshnikov[c] and D. Sundholm[b]

Check for updates

Cite this: *Phys. Chem. Chem. Phys.*, 2019, **21**, 18495

Calculating rate constants for intersystem crossing and internal conversion in the Franck–Condon and Herzberg–Teller approximations†

Rashid R. Valiev,[*ab] Victor N. Cherepanov,[a] Rinat T. Nasibullin,[a] Dage Sundholm[c] and Theo Kurtén[b]

Check for updates

Cite this: *Phys. Chem. Chem. Phys.*, 2020, **22**, 22314

First-principles calculations of anharmonic and deuteration effects on the photophysical properties of polyacenes and porphyrinoids

R. R. Valiev,[*ab] R. T. Nasibullin,[b] V. N. Cherepanov,[b] G. V. Baryshnikov,[cd] D. Sundholm,[a] H. Ågren,[c] B. F. Minaev[cd] and T. Kurtén[a]

Check for updates

Cite this: *Phys. Chem. Chem. Phys.*, 2021, **23**, 6344

Received 19th January 2021,
Accepted 9th March 2021

Fast estimation of the internal conversion rate constant in photophysical applications

R. R. Valiev,[*ab] R. T. Nasibullin,[c] V. N. Cherepanov,[c] A. Kurtsevich,[c] D. Sundholm[a] and T. Kurtén[a]

Check for updates

Cite this: *Phys. Chem. Chem. Phys.*, 2023, **25**, 6406

Internal conversion rate constant calculations considering Duschinsky, anharmonic and Herzberg–Teller effects†

R. R. Valiev,[*abcd] B. S. Merzlikin,[c] R. T. Nasibullin,[d] A. Kurtzevitch,[d] V. N. Cherepanov,[d] R. R. Ramazanov,[a] D. Sundholm[a] and T. Kurtén[a]

Check for updates

Cite this: *Phys. Chem. Chem. Phys.*, 2025, **27**, 16853

The role of X–H bonds (X = C, N and O) in internal conversion processes: dibenzoterrylene as an example†

Rashid R. Valiev,[*a] Boris S. Merzlikin,[b] Rinat T. Nasibullin,[a] Dage Sundholm[a] and Theo Kurtén[a]

Rinat Nasibullin

PHOTOPHYSICAL PROPERTIES (2012-)

Rashid Valiev

Rinat Nasibullin

Lucie Tučková

Check for updates

Cite this: *J. Mater. Chem. C*, 2022, **10**, 4894

Influence of perhalophenyl groups in the TADF mechanism of diphosphino gold(I) complexes†

Inés Soldevilla,[a] Aimara Garcia-Camacho,[a] Rinat T. Nasibullin,[b] M. Elena Olmos, [a] Miguel Monge, [a] Dage Sundholm, [c] Rashid R. Valiev,[d] José M. López-de-Luzuriaga [a]*[a] and María Rodríguez-Castillo [a]*[a]

Check for updates

Cite this: *Phys. Chem. Chem. Phys.*, 2022, **24**, 18713

On the origin of the inverted singlet–triplet gap of the 5th generation light-emitting molecules†

Lucie Tučková, [a] Michal Straka,[a] Rashid R. Valiev [b] and Dage Sundholm [b]*[b]

Check for updates

Cite this: *Chem. Sci.*, 2023, **14**, 3873

All publication charges for this article

Gold(I)-containing light-emitting molecules with an inverted singlet–triplet gap†

Daniel Blasco, [ab] Rinat T. Nasibullin,[c] Rashid R. Valiev[a] and Dage Sundholm [a]*[a]

Check for updates

Cite this: *Phys. Chem. Chem. Phys.*, 2024, **26**, 5922

Experimental and computational studies of the optical properties of 2,5,8-tris(phenylthiolato)heptazine with an inverted singlet–triplet gap†

Daniel Blasco, [a]*[a] Rinat T. Nasibullin,[b] Rashid R. Valiev,[b] Miguel Monge, [a] José M. López-de-Luzuriaga [a] and Dage Sundholm [a]*[b]

Check for updates

Cite this: *J. Mater. Chem. C*, 2024, **12**, 13255

Improving the quantum yield of luminescence for three-coordinated gold(I) TADF emitters by exploiting inversion symmetry and using perhaloaryl ligands†

Inés Soldevilla,[a] Abdel Ghafour El-Hachimi, [a] Ruslan Ramazanov,[c] Rashid R. Valiev,[b] M. Elena Olmos, [a] Miguel Monge, [a] Dage Sundholm, [b] María Rodríguez-Castillo [a]*[a] and José M. López-de-Luzuriaga [a]*[a]

Check for updates

Cite this: *Inorg. Chem. Front.*, 2026, **13**, 377

The role of the electron density of the acceptor in efficient diphenylphosphino-gold(I) TADF emitters

Oliver Baltar, [a] Inés Soldevilla,[a] Rinat T. Nasibullin,[b] Rashid R. Valiev,[b] M. Elena Olmos, [a] Miguel Monge, [a] Dage Sundholm, [b] María Rodríguez-Castillo [a]*[a] and José M. López-de-Luzuriaga [a]*[a]

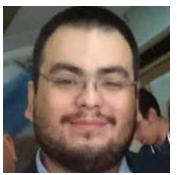
Daniel Blasco

Miguel Monge

Spaniards and Latin Americans

Fernando Mendizabal (Chile)

Alvaro Muñoz Castro (Chile)

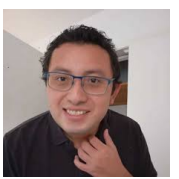


Carlos Orellana (Chile)

Sebastian Miranda-Rojas (Chile)

Raul Mera (Chile)

Jesus Muñiz (Mexico)



Mesías Orozco-Ic (Mexico)

Filiberto Montiel (Mexico)

Daniel Blasco (Spain)

Miguel Monge (Spain)

Felix Reboiro (Spain)

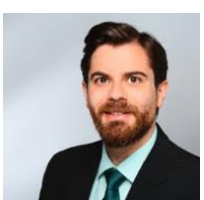
ALEMANITOS

Raphael Berger

Yannick Franzke

Robert Send

Jonas Greiner



Kevin Reiter

Nina Winter

Mathias Pabst

Antonia Rabe

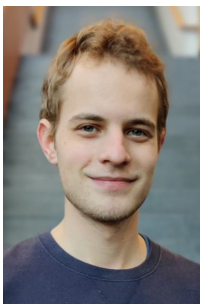
SOME STUDENTS

Isaac Benkyi

Markus Rauhalahti

Cong Wang

Usman Ahmed



Hugo Åström

Nergiz Özcan

Qian Wang

Atif Mahmood

Ying-Chan Lin

Dou Du

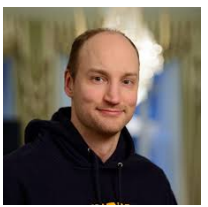
SOME COWORKERS

Hassan Rabaâ
(Morocco)

Martin Kaupp
(Germany)

Michael Patzschke

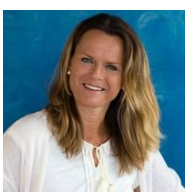
Michal Straka



Susi Lehtola

Juha Vaara

Janne Pesonen



Susanne Wiedmer

Yavus Dede
(Türkiye)

Hiroshi Shinokubo
(Japan)

Harapriya Rath
(India)

BEFORE ENDING

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.

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

Helsingin Yliopistokiinteistöt Oy's turnover in 2024 was 68.0 M€ consisting entirely of rental income. It is an increase of 6.4% from 2023. The company's result was 22.2 M€. Why?

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 groups publishing the scientific articles.

If the research groups could keep a significant share of the JUFO funding, PhD students could contribute to their own salary by writing scientific articles.

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 Chemistry Department.

The reason was not bad performance but other units at the Chemistry 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 little boy supporting the weak.

I would like to thank all coworkers, without their efforts I would have had much less to talk about today.

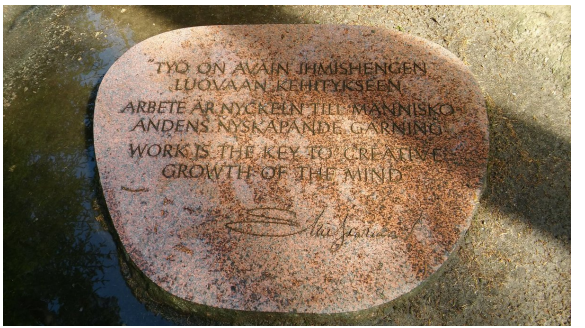
I have had young coworkers who turned into skillful researchers and it happens remarkably fast.

Chemists must allow themselves to do research in areas that do not lead to a product in the foreseeable future.

Basic research contributes to future technology and pushes the boundaries of our knowledge.

I end here.

Wovon man nicht sprechen kann, darüber muss man schweigen
Whereof one cannot speak, thereof one must be silent
(Ludwig Wittgenstein)



Work is the Key to Creative Growth of the Mind
Arbete är Nyckeln till Människoandens Nyskapande Gärning
Työ on Avain Ihmishengen Luovaan Kehitykseen
(Eliel Saarinen)

I may never find all the answers
I may never understand why
I may never prove
What I know to be true
But I know that I still have to try
(Dream Theater in The Spirit Carries on)