Academic portfolio 7.3.2024

1) Basic Information

- **PERSONAL AND CONTACT INFORMATION**

Thomas Olof Sebastian Sandberg
Gamla Tavastlandsvägen 110 B 37
FIN-20540 Åbo, Finland
+358-(0)40-539 4636
thomas.sandberg@abo.fi
Google Scholar Profile
Born 28.3.1978 in Turku
Children 2007 and 2009

- **EDUCATION AND DEGREES**

Åbo Akademi University, Turku, Finland

Teacher Qualification in Higher Education **21.4.2020**

Docent in Computational Chemistry **15.1.2020**

Ph.D. in Quantum Chemistry **18.6.2013**
Thesis: "Computational chemistry studies on wood-derived lignans"
Major: Quantum Chemistry and Molecular Spectroscopy
Minor: Mathematics and University Education

Ph.L. in Quantum Chemistry **15.9.2009**
Thesis: "Computational chemistry studies on lignans"
Major: Quantum Chemistry and Molecular Spectroscopy
Minor: Mathematics and University Education

M.Sc. in Chemistry **13.9.2005**
Thesis: "Quantum chemical calculations on acidity and basicity of some toluene derivatives"
Major: Chemistry (A)
Minor: Mathematics (A), Physics (A) and Education

B.Sc. in Chemistry **31.5.2001**
Thesis: "A study in symmetry groups"

Katedralskolan i Åbo, Turku, Finland
Matriculation exam **31.5.1997**

- **CURRENT POSITION**

University Lecturer (1.8.22) in Physical Chemistry at *Åbo Akademi University* **08.2015–Present**

- Lectured courses in chemistry and spectroscopy at basic, intermediate and advanced level as well as instructed in computer exercises and lab work
  - Developed overall course structure and teaching material and administered all grades in Atomic structure and chemical properties.

- **PREVIOUS WORK EXPERIENCE**

Åbo Akademi University, Turku, Finland
Teaching Assistant in Chemistry/**University Teacher** in Molecular Modelling **10.2014–07.2015**
- Instructed first-year-students in planning, lab work and documentation of open lab work in General Chemistry (part time, 50%)
- Lectured in Molecular Modelling and instructed in computer exercises (part time, 30–47%).

Post-doctoral grant researcher (12 months, see details below) **2014–05.2015**

Post-doctoral researcher in Physical Chemistry (2 months) **11–12.2013**

Co-ordinator of chemistry study reform (4 months) **07–10.2013**
- Realized regular teacher meetings (29 times/18 months) for planning and follow-up of the chemistry education.
- Strengthened the team spirit between the five subjects of chemistry at ÅAU and the teaching personnel.
- Presented a suggestion to a reform of the bachelor level studies in chemistry.

PhD student in Physical Chemistry (part time, 33%, 6–9 months/year) **2011–06.2013**

Grant research funding for PhD studies (38 months, see details below) **01–08.2006**
04.2011–06.2013

Teaching Assistant in Physical Chemistry (2–3 months/year) **2006–2012**
- Prepared chemicals, apparatus and teaching material, instructed in lab work and report writing, and administered all grades (2011–2012).
- Co-supervised B.Sc. Thesis (2008).
- Constructed and administered three virtual courses at the course platform Moodle.

Graduate School of Computational Chemistry and Molecular Spectroscopy (LASKEMO), Finland
PhD student (9 months/year) **09.2006–2010**

Resource Center for Mathematics, Science and Technology at School, Finland
Research Contact **2008–Present**

Åbo Akademi University, Turku, Finland
Non-permanent Teacher in Molecular Modelling **2006–2010**
- Instructed in computer exercises (171 h) and lectured (12 h, 2010).

Non-permanent Teacher for pre-university students ("abiturienter") **2006–2009**
- Instructed in computer exercises.

Research Assistant in Physical Chemistry (4 months) **2005**

Non-permanent Teacher in Propaedeutic (Preparatory) Chemistry (282 h) **2001–2005**
- Developed overall course structure and teaching material and administered all grades.

Private Teacher in Chemistry and Mathematics (high school level) **2001–2005**

Högstadiet (senior-level compulsory) Sankt Olofsskolan i Åbo, Turku, Finland
Supply Teacher in Mathematics, Physics, Chemistry and Computer Science **2000–2004**

Åbo Akademi University, Turku, Finland
Research Assistant in Physics (4 months) **1998–2000**

Patenttitoimisto Kari Pirhonen OY
Translator of patent applications, mainly Finnish–Swedish **1997–2005**

• LANGUAGE SKILLS

Swedish – native language
Finnish and **English** – speak fluently and read/write with high proficiency
German – speak, read, and write with basic competence.

2) Research and Scientific Activities

- **EXPERIENCE IN RESEARCH AND RESEARCH COOPERATION**

Computational chemistry is of utmost importance in chemistry research today. A central shortcoming in development of new molecules is the proper characterization of new, molecular structures at atomic level with accurate quantum chemical methods. The key factor often affecting the molecular minimum energy configuration is the solvent. In molecular dynamics simulations the solvent molecules are explicitly present, thereby defining a more accurate description on how the solvent molecules affect the molecular conformation. My research area has mainly comprised **molecular dynamics simulations** and **quantum chemical structural optimizations**.

Supporting experimental research is one of the main tasks for a computational chemist. Because of this interdisciplinary nature, I have recently been collaborating with the following laboratories at Åbo Akademi University:

- Prof. Dmitry Murzin's group in Industrial Chemistry and Reaction Engineering
- Prof. Reko Leino's group in Organic Chemistry
- Prof. Johan Bobacka's group in Analytical Chemistry
- Prof. Jessica Rosenholm's group in Pharmaceutical Sciences

Since the retirement of Prof. Matti Hotokka in 2014, I am responsible for the computational chemistry research and education at the Laboratory of Physical Chemistry. During the year 2014, I worked as a postdoctoral grant researcher in collaboration with prof. Aurora Clark's group at Washington State University in Pullman, where I conducted research visits in June 2014 and in July 2015.

- **PUBLICATIONS**

A Peer-reviewed scientific articles and manuscripts

23) Ida Mattsson, Johanna Majoinen, Manu Lahtinen, Thomas Sandberg, Anna Fogde, Tiina Saloranta-Simell, Orlando Rojas, Olli Ikkala, Reko Leino*, "Stereochemistry-dependent thermotropic liquid crystalline phases of monosaccharide-based amphiphiles", *Soft Matter*, **2023**, *19*, 8360–8377, **DOI:** https://doi.org/10.1039/D3SM00939D.

22) Anna Fogde, Emil Rosqvist, Trung-Anh Le, Jan-Henrik Smått, Thomas Sandberg, Tan-Phat Huynh*, "A Further Study on Calcium Phosphate Gardens Grown from the Interface of κ-Carrageenan-based Hydrogels and Counterion Solutions", *ChemPlusChem*, **2023**, *88*, e202200426, **DOI:** 10.1002/cplu.202200426.

21) Anna Fogde, Syeda Qudsia, Trung-Anh Le, Thomas Sandberg, Tan-Phat Huynh*, "(Calcium-phosphate)/carrageenan gardens grown from the gel/liquid interface", *ChemSystemsChem*, **2021**, *3*, e2000064, **DOI:** 10.1002/syst.202000064.

20) Anna Fogde, Berit Kurtén, Thomas Sandberg, Tan-Phat Huynh*, "Colorimetric Hydrogel from Natural Indicators – a Tool for Electrochemistry Education", *The Journal of Chemical Education*, **2020**, *97*, 3702–3706, **DOI:** 10.1021/acs.jchemed.0c00440.

19) Alexander Sidorenko, Anna Kravtsova, Päivi Mäki-Arvela, Atte Aho, Thomas Sandberg, I.V. Il'ina, Nikolai Li-Zhulanov, D.V. Korchagina, Konstantin P. Volcho, Nariman F. Salakhutdinov, Dmitry Yu. Murzin; Vladimir E. Agabekov*, "Synthesis of isobenzofuran derivatives from renewable 2-carene over halloysite nanotubes", *Molecular Catalysis*, **2020**, *490*, 110974, **DOI:** 10.1016/j.mcat.2020.110974.

18) Mathias Laluc, Päivi Mäki-Arvela, Andreia F. Peixoto, Nikolai Li-Zhulanov, Thomas Sandberg, Nariman Salakhutdinov, Konstantin Volcho, Christina Freire, Alexander Yu. Sidorenko, Dmitry Yu. Murzin*, "Catalytic synthesis of bioactive 2H-chromene alcohols from (-)-isopulegol and acetone on sulphonated clays", *Reaction Kinetics, Mechanisms and Catalysis*, **2020**, *129*, 627–644, **DOI:** 10.1007/s11144-020-01740-9. **OPEN ACCESS.**

17) Alexander Sidorenko, Nikolai Li-Zhulanov, Päivi Mäki-Arvela, Thomas Sandberg, Anna Kravtsova, Andreia Peixoto, Cristina Freire, Konstantin Volcho, Nariman Salakhutdinov, Vladimir Agabekov, Dmitry Murzin*, "Stereoselectivity inversion by water addition in the –SO3H catalyzed tandem Prins-Ritter reaction for synthesis of 4-amidotetrahydropyran derivatives", *ChemCatChem*, **2020**, *12*, 1–6, **DOI:** 10.1002/cctc.202000070.

16) Nikolai Li-Zhulanov, Päivi Mäki-Arvela, Mathias Laluc, Andreia F. Peixoto, Ekaterina Kholkina, Thomas Sandberg, Atte Aho, Konstantin Volcho, Nariman Salakhutdinov, Christina Freire, Alexander Yu. Sidorenko, Dmitry Yu. Murzin*, "Prins cyclization of (-)-isopulegol with benzaldehyde for production of chromenols over organosulfonic clays", *Molecular Catalysis*, **2019**, *478*, 110569, **DOI:** 10.1016/j.mcat.2019.110569.

15) E. Kolobova, P. Mäki-Arvela, A. Pestryakov, E. Pakrieva, L. Pascual, A. Smeds, J. Rahkila, T. Sandberg, J. Peltonen, D. Yu. Murzin*, "Reductive amination of ketones with benzylamine over gold supported on different oxides", *Catalysis Letters*, **2019**, *149*, 3432–3446, **DOI:** 10.1007/s10562-019-02917-1. **OPEN ACCESS.**

14) Alvaro Gonzalez-Vogel, Anna Fogde, Claudia Crestini, Thomas Sandberg, Tan-Phat Huynh, Johan Bobacka*, "Molecularly imprinted conducting polymer for determination of a condensed lignin marker", *Sensors and Actuators B: Chemical*, **2019**, *295*, 186–193, **DOI:** 10.1016/j.snb.2019.05.011. **OPEN ACCESS.**

13) Thomas Sandberg*, Christian Weinberger, Jan-Henrik Smått, "Molecular Dynamics on Wood-Derived Lignans Analyzed by Intermolecular Network Theory", *Molecules,* **2018**, *23*(8), 1990, **DOI:** 10.3390/molecules23081990. **OPEN ACCESS.**

12) Christian Weinberger*, Marc Hartmann, Sai Ren, Thomas Sandberg, Jan-Henrik Smått, Michael Tiemann, "Selective Pore Filling of Mesoporous CMK-5 Carbon Studied by XRD: Comparison between Theoretical Simulations and Experimental Results", *Microporous & Mesoporous Materials,* **2018**, *266*, 24–31, **DOI:** 10.1016/j.micromeso.2018.02.035 + poster, **DOI:** 10.13140/RG.2.2.11102.54084. **OPEN ACCESS.**

11) Thomas Sandberg*, Christian Weinberger, Didem Şen Karaman, Jessica M. Rosenholm, "Modeling of a hybrid Langmuir adsorption isotherm for describing interactions between drug molecules and silica surfaces", *Journal of Pharmaceutical Sciences,* **2018**, *107*, 1392–1397, **DOI:** 10.1016/j.xphs.2017.12.025 + poster, **DOI:** 10.13140/RG.2.2.21693.15847.

10) Thomas Sandberg*, Patrik Eklund,
"The effect of density functional dispersion correction (DFT-D3) on lignans", *Computational and Theoretical Chemistry,* **2015**, *1067*, 60–63, **DOI:** 10.1016/j.comptc.2015.05.023.

9) Otto Långvik, Thomas Sandberg, Johan Wärnå, Dmitry Yu. Murzin, Reko Leino*,
"One-pot Synthesis of (R)-2-Acetoxy-1-indanone from 1,2-Indanedione Combining Metal Catalyzed Hydrogenation and Chemoenzymatic Dynamic Kinetic Resolution", *Catalysis Science & Technology,* **2015**, *5*, 150–160, **DOI:** 10.1039/C4CY01099J.

8) Thomas Sandberg, Patrik Eklund, Matti Hotokka,
"Computational Chemistry Studies of LIGNOLs", In *Applied Parallel and Scientic Computing*, Manninen, P.; Öster, P., Ed., volume 7782 of *Lecture Notes in Computer Science*, pp. 553–557. Springer Berlin Heidelberg, **2013**, **DOI:** 10.1007/978-3-642-36803-5_45.

7) Yury Brusentsev, Thomas Sandberg, Matti Hotokka, Rainer Sjöholm, Patrik Eklund*, "Synthesis and structural analysis of sterically hindered chiral 1,4-diol ligands from the lignan hydroxymatairesinol", *Tetrahedron letters,* **2013**, *54*(9), 1112–1115, **DOI:** 10.1016/j.tetlet.2012.12.066. **OPEN ACCESS.**

6) Thomas Sandberg*, Patrik Eklund, Matti Hotokka, "Conformational Solvation Studies of LIGNOLs with Molecular Dynamics and Conductor-Like Screening Model", *International Journal of Molecular Sciences,* **2012**, *13*(8), 9845-9863, **DOI:** 10.3390/ijms13089845. **OPEN ACCESS.**

5) Thomas Sandberg, Yury Brusentsev, Patrik Eklund and Matti Hotokka*, "Structural analysis of sterically hindered 1,4-diols from the naturally occurring lignan hydroxymatairesinol. A quantum chemical study" *International Journal of Quantum Chemistry,* **2011**, *111*(15), 4309–4317, **DOI:** 10.1002/qua.22965.

4) Thomas Sandberg, Matti Hotokka*, "Conformational analysis of hydroxymatairesinol in aqueous solution with molecular dynamics", *Journal of Computational Chemistry,* **2009**, *30*(16), 2666–2673 (+ cover page!), **DOI:** 10.1002/jcc.21293.

3) Thomas Sandberg, Jessica Rosenholm, Matti Hotokka*, "The molecular structure of disulfiram and its complexation with silica. A quantum chemical study", *Journal of Molecular Structure (THEOCHEM),* **2008**, *861*(1–3), 57–61, **DOI:** dx.doi.org/10.1016/j.theochem.2008.04.007.

2) Heidi Markus, Arie J. Plomp, Thomas Sandberg, Ville Nieminen, Johannes H. Bitter, Dmitry Yu. Murzin* "Dehydrogenation of Hydroxymatairesinol to Oxomatairesinol over Carbon Nanofibre-Supported Palladium Catalysts", *Journal of Molecular Catalysis A,* **2007**, *274*(1–2), 42–49,
DOI: dx.doi.org/10.1016/j.molcata.2007.04.025.

1) Björn Granqvist, Thomas Sandberg, Matti Hotokka*, "Adsorption of organic probes on silica through Lewis interactions: A comparison of experimental results and quantum chemical calculations", *Journal of Colloid and Interface Science,* **2007**, *310*(2), 369–376, **DOI:** dx.doi.org/10.1016/j.jcis.2007.02.008.

B Non-refereed scientific articles (poster abstracts)

Christian Weinberger, Marc Hartmann, Sai Ren, Thomas Sandberg, Jan-Henrik Smått, Michael Tiemann, Selective Pore Filling of Mesoporous CMK-5 Carbon Studied by XRD Theoretical Simulations and Experimental Results
In *30th German Zeolite Conference, Kiel, Germany, 28.2–2.3.2018. 1 p.* **(2018)**

Thomas Sandberg, Christian Weinberger, Didem Şen Karaman, Jessica Rosenholm,
Describing Drug Molecule Silica Interactions by Modeling of Hybrid Langmuir Adsorption Isotherms
In *1st International Symposium on Quantum Technology, Aberdeen, Scotland, 24–27.6.2018. 1 p.*, In *30th German Zeolite Conference, Kiel, Germany, 28.2–2.3.2018. 1 p.* **(2018)**

Thomas Sandberg, Patrik Eklund and Matti Hotokka,
Conformational Solvation Studies of LIGNOLs with Molecular Dynamics and COSMO
In *Winter School in Theoretical Chemistry 2013, Helsinki, 16–19.12.2013. 1 p.* **(2013)**, In *17th International Workshop on Quantum Systems in Chemistry and Physics, Turku, 19–25.8.2012. 1 p.,* In *14th International Congress of Quantum Chemistry, Boulder, Colorado, USA*, 25–30.6.2012. *1 p.,* In *FunMat Annual Symposium Posters 23.5.2012. 1 p.* **(2012)**

T. Sandberg, H. Markus, V. Nieminen, D.Yu. Murzin,
Dehydrogenation of Hydroxymatairesinol to Oxomatairesinol
In *Winter School in Theoretical Chemistry 2012, Helsinki, 17–20.12.2012. 1 p.*, In *17th International Workshop on Quantum Systems in Chemistry and Physics, Turku, 19–25.8.2012. 1 p.* **(2012)**

Thomas Sandberg, Gun Hedström, Björn Granqvist, J.B. Rosenholm, Matti Hotokka,
Interaction of benzyl probes with silica in cyclohexane. *Ab initio* calculations, adsorption and microcalorimetry
In *Winter School in Theoretical Chemistry 2012, Helsinki, 17–20.12.2012. 1 p.*, In *17th International Workshop on Quantum Systems in Chemistry and Physics, Turku, 19–25.8.2012. 1 p.* **(2012)**

Thomas Sandberg, Jessica Rosenholm, Matti Hotokka,
Interactions between Antabus® and silica surfaces
In *Winter School in Theoretical Chemistry 2012, Helsinki, 17–20.12.2012. 1 p.*, In *17th International Workshop on Quantum Systems in Chemistry and Physics, Turku, 19–25.8.2012. 1 p.* **(2012)**

Thomas Sandberg, Yury Brusentsev, Patrik Eklund and Matti Hotokka
Structural analysis of sterically hindered 1,4-diols from the naturally occurring lignan HMR
In *17th International Workshop on Quantum Systems in Chemistry and Physics, Turku, 19–25.8.2012. 1 p.,* In *14th International Congress of Quantum Chemistry, Boulder, Colorado, USA*, 25–30.6.2012. *1 p.* **(2012)**, In *Winter School in Theoretical Chemistry 2011, Helsinki, 12–15.12.2011. 1 p.*, In *FunMat Annual Symposium 24.8.2011. 1 p.* **(2011)**

Thomas Sandberg, Matti Hotokka,
Conformational analysis of hydroxymatairesinol in aqueous solution with molecular dynamics
In *Winter School in Theoretical Chemistry 2013, Helsinki, 16–19.12.2013. 1 p.* **(2013)**, In *17th International Workshop on Quantum Systems in Chemistry and Physics, Turku, 19–25.8.2012. 1 p.* **(2012)**, In *Nanoscience Days 2009, Jyväskylä. 1 p.*, In *13th ICQC International Congress of Quantum Chemistry, Helsinki, 22-27.6.2009. 1 p.,* In *FunMat Seminar 3.3.2009. 1 p.* **(2009)**

Björn Granqvist, Thomas Sandberg, Matti Hotokka
Adsorption of organic probes on silica through Lewis interactions.
A comparison of experimental results and quantum chemical calculations
In *Graduate School of Materials Research Seminar 23.5.2006. 1 p.* **(2006)**

C Scientific books (monographs)

QSCP-XVII, International Workshop on Quantum Systems in Chemistry and Physics
ABSTRACTS AND PROGRAM, August 19–25, **2012**, Turku, Finland
Edited by T. Sandberg and J.-H. Smått, ISBN 978-952-12-2761-5

D Publications intended for professional communities (teaching material)

Thomas Sandberg and Anna Fogde, *Datorövningar i Atomstruktur och kemiska egenskaper,* 10 pp., **2015**.

Thomas Sandberg and Matti Hotokka, *Atomstruktur och kemiska egenskaper,* 147 pp., **2015**.

Thomas Sandberg and Gun Hedström, *Fysikalisk kemi, Laborationer B*, 26 pp., **2011**.

Thomas Sandberg and Gun Hedström, *Fysikalisk kemi, Laborationer A*, 44 pp., **2011**.

Thomas Sandberg and Matti Hotokka, *Övningar i modellering*, 38 pp., **2008**.

Thomas Sandberg, *Övningar för Abikurs i kemi. Molekylmodellering*, **2008**.

Matti Hotokka and Thomas Sandberg, *Övningar i modellering*, 40 pp., **2007**.

E Publications intended for the general public, linked to the applicant's research

Thomas Sandberg, Guest column about grant research in *Meddelanden från Åbo Akademi*, **2014**, *Nr 3, April*, p. 35. ISSN 2341-9644. **OPEN ACCESS.**

G Theses

Thomas Sandberg, *Computational chemistry studies on wood-derived lignans,* PhD thesis, Åbo Akademi University, **2013**. **OPEN ACCESS.**

Thomas Sandberg, *Beräkningskemiska studier av lignaner*, PhL thesis, Åbo Akademi University, **2009**.

Thomas Sandberg, *Kvantkemiska beräkningar av syra-basegenskaper hos några toluenderivat*, MSc thesis, Åbo Akademi University, **2005**.

Thomas Sandberg, *En studie i symmetrigrupper med fördjupning i rymdgrupp nr. 53*, BSc thesis, Åbo Akademi University, **2001**.

- **EXPERT ASSESSMENTS**

Member of the examination boards of nine doctoral dissertations, *ÅAU*: Qian Xu, Petri Sirviö, Didem Sen Karaman, Martin Slotte, Tina Gulin-Sarfraz, Anne Norström, Meheretu Dirbeba, Matilda Kråkström, Mahlet Zerihun Tamirat **2016–21**

Member of the pedagogical committee of two test lectures, *ÅAU*: Mika Jokinen and Adriana Ferancovas **2004, 2019**

Pre-examiner of the PhD thesis of Mario Öeren and Irina Osadchuk, *Tallinn University of Technology* **2015–17**

Fourteen referee assignments for *Journal of Computational Chemistry*, *Physica Scripta*, *Journal of Computational Chemistry and Molecular Modelling, Axioms, Mathematics* and *Symmetry* **2014** **2018–19**

- **RESEARCH FUNDING – HONOURS AND SCIENTIFIC GRANTS**

Åbo Akademis jubileumsfond 1968 (mobility grant)	**→ 2024**
Ellida och Tor Magnus Ljungbergs stipendiefond	**2011–12, 2014, 2016–23**
Berndt Olof Grönbloms fond	**2011, 2013–14, -19, -21, -23**
Chancellor's travel mobility grant "Guldkanten"	**→ 2022**
Edgar Grönbloms stipendiefond för lärare (research visit)	**2014**
Alfred Kordelins stiftelse, Gust. Komppas fond (research visit)	**→ 2015**
Svenska Tekniska Vetenskapsakademien i Finland (research visit)	**2014–15, 2019**
Victoriastiftelsen (9+12+5+12 months)	**2011–14**
Magnus Ehrnrooths stiftelse (1+6 months)	**2006, -13**
Stiftelsens för Åbo Akademi forskningsinstitut (5+6+12 months)	**2006, -12, -14**

- **COMMISSIONS OF TRUST**

1st International Symposium on Quantum Technology, Aberdeen, Scotland

Member of the **Scientific Committee**. **2018**

17th International Workshop on Quantum Systems in Chemistry and Physics, QSCP, Turku

Was included in the **Local Organizing Committee**. Administered the **Conference E-mails**. Edited the **Abstract Book**. Organized the **Poster Sessions**. Served as Master of Music at the **Award Ceremony Banquet**. **2012**

9th International Conference on Electrokinetic Phenomena, ELKIN, Turku, Finland

Organized the **Accompanying Persons Programme**. **2010**

- **CONFERENCES AND COURSES**

Winter Schools in Theoretical Chemistry at University of Helsinki, Finland

- 32th "Current Trends in Electronic Structure Theory Methods" 12–15.12.**2016**
- 31th "Computational Biochemistry" 14–17.12.**2015**
- 30th "Theoretical f-Element Chemistry" 15–18.12.**2014**
- 29th "Theoretical Spectroscopy" 16–19.12.**2013**, 2 poster presentations.
- 28th "Nuclear motion in molecules" 17–20.12.**2012**, 3 poster presentations.
- 27th "Excited State Properties" 12–15.12.**2011**, 1 poster presentations.
- 26th "Accurate Molecular Structure" 13–16.12.**2010**
- 25th "Chemical Bonding" 14–17.12.**2009**
- 24th "Reactions on Surfaces" 10–12.12.**2008**
- 23rd "Actinide Chemistry" 10–14.12.**2007**
- 22nd "Astrochemistry" 11–14.12.**2006**
- 21th "Nanophotonics" 7–9.12.**2005**

"*Workshop on Physical Chemistry Education"* in Gothenburg, Sweden, 6–7.3.**2024**, oral presentation.
"*1st International Symposium on Quantum Technology*" in Aberdeen, Scotland, 24–27.6.**2018**, online participation with poster, member of the scientific committee.
"17th International Workshop on Quantum Systems in Chemistry and Physics" in Turku, 19–25.8.**2012**, 6 poster presentations.
"14th International Congress of Quantum Chemistry" in Boulder, Colorado, USA, 25–30.6.**2012**, 2 poster presentations.
"PARA 2012: Workshop on State-of-the-Art in Scientific and Parallel Computing" in Helsinki, 10–13.6.**2012**, oral presentation.
"Center of Excellence for Functional Materials Annual Seminar" in Turku 23.5.**2012**, poster presentation.
"Center of Excellence for Functional Materials Annual Symposium" in Turku "Materials for the future" 24–25.8.**2011**, poster presentation.
"DEISA PRACE Symposium" in Helsinki 13–14.4.**2011**
"Nanoscience Days 2009" in Jyväskylä 29–30.10.**2009**, poster presentation.
"The LasKeMo Days 2009" in Strandbo, Nauvo 12–13.10.**2009**, oral presentation.
"The 13th International Congress of Quantum Chemistry" in Helsinki "Science at the Summer Solstice" 22–27.6.**2009**, poster presentation.
"Joint COMP-Laskemo/CMS symposium" in Otaniemi, "van der Waals interactions" 24.4.**2008**
"The 17th Jyväskylä Summer School "Computational Nanoscience", 5 sp, 13–24.8.**2007**
"Joint Graduate School Seminar" at Hanasaari, Espoo, "Phys. and Chem. of Materials: Towards Nano" 8–9.12.**2006**, oral presentation.

Courses at CSC, the IT Center for Science, Espoo, Finland

- "Schrödinger Maestro Materials Science Hands-on Workshop", 17.1.**2020**, remotely via Zoom.
- "Schrödinger Maestro 11 - New Interface", 26.10.**2016**, remotely via Adobe Connect Pro.
- "Gromacs 5" 23.11.**2015**
- "Schrödinger computational chemistry day" 12.11.**2015**
- "CSC Spring School in Computational Chemistry" 18–21.3.**2014**
- "Using Accelrys Materials Studio" 4–5.2.**2014**
- "CSC Spring School in Computational Chemistry" 5–9.3.**2012**, 2 poster presentations.
- "Elmer Intensive Course" 7.9.**2011**
- "Computational Resources BoF" 28.3.**2011**
- "Fortran 95" 8–9.10.**2008**
- "Sybyl Training Course" 26–27.2.**2008**
- "CPMD, Car-Parinello Molecular Dynamics" 24–25.10.**2006**
- "Turbomole, basics and advanced" 28–29.9.**2006**

3) Teaching and Supervision

- **PEDAGOGICAL TRAINING**

Åbo Akademi University, Turku, Finland

- Higher Education Learning Lab – HELLA, 60 credits, **2020**
  - University teacher education, 25 credits, **2009–2018**
  - Basic studies in educational leadership, 29 credits (grade 5/5), **1998–2018**

HHÅA's autumn conference on teaching environment, 25.11.**2016**, 23.10.**2015**
Mini conference on teaching and examination methods at IPL, 16.5.**2014**
Mini conferences VIII–XII in course development, **2008–2012**
Didactics day in Turku, 5.10.**2009**, 1.10.**2007**

- **EXPERIENCE IN TEACHING AND SUPERVISION**

Since October 2014, I have continuously been teaching at undergraduate university level in general chemistry as well as molecular modelling, including lecturing, instructing in lab work, examination and administration of grades. I am responsible for two of the basic level chemistry courses designed during the reform in 2013 (see below) and teaching in five other courses at Bachelor level.

Until 2013, I was mainly teaching at undergraduate university level as laboratory assistant in physical chemistry at ÅAU. The work constituted supervision, both in the laboratory and when the students were writing reports, which is an important part of the laboratory courses.

I have also given the courses in preparatory chemistry for students at ÅAU lacking basic knowledge in chemistry when beginning their university studies.

In addition to this, I have supervised computer exercises and been teaching in molecular modelling at ÅAU since 2006. In 2008, I was co-supervising the Bachelor thesis of Tina Gulin, and in 2015 the Master's thesis of Anna Fogde, which also resulted in an A-publication. Since 2020, I was the supervisor of Anna Fogde's PhD studies, which resulted in a thesis that was defended in August 2023. Additionally, I have supervised the Bachelor thesis of Nicolas Kraufvelin that was finished in 2022. More details can be seen in the enclosed teaching portfolio.

- **DEVELOPMENT OF TEACHING MATERIAL AND USE OF EDUCATIONAL TECHNOLOGY**

For me as a computational chemist, IT in teaching goes without saying, still without being an end in itself. There are two acceptable alternatives for visualizing molecular structures: plastic models and modelling programs, the latter often more easily accessible and even free in many cases. Some of the software I have been using both for research and for teaching based upon research, is seen in the computer skills below. A lot of the computational software has implemented visualizing modules. Other teaching material (compendia, Moodle etc.) can be seen in the enclosed teaching portfolio.

- **COMPUTER SKILLS**

Windows, Linux, Mas OS X
Programming: C and Fortran 77 and 90/95
LaTeX (progr. language for typesetting of text)
HTML programming: http://web.abo.fi/~tsandber
Xfig (grafics program)
Gnuplot (data plotting)
Gromacs (molecular dynamics)
GAMESS, Turbomole (quantum chemistry)

- **DEVELOPMENT OF TEACHING**

During the year 2013, I was co-ordinating a strategy group of five chemistry teachers at ÅAU with the mission to initiate a closer collaboration between the subjects in chemistry teaching. We introduced regular teacher meetings for planning and follow-up of the chemistry education. The aims of the project contained a strengthening of the team spirit between the five subjects of chemistry at ÅAU and the teaching personnel, which we attained excellently. As a conclusion of the project, we presented a suggestion to a continuation of the collaboration within the basic funding as well as a reform of the bachelor level studies in chemistry. The new structure was implemented in the autumn of 2015.

- **COURSE EVALUATIONS AND OTHER QUALITY EVALUATION**

The course *Atomic structure and chemical properties* was accomplished for the first time during the autumn of 2015. I was responsible for the course in a team of five teachers from the Laboratories of Inorganic and Physical Chemistry at ÅAU. We had a well working spirit of community between the teachers with weekly planning and evaluation meetings. Because of structural reasons, there were only students in the study program of Natural sciences in 2015, but the course was all the time planned for the fourfold amount of students attending from year 2016. In the course last year, 78 students passed.

As in the course *General chemistry and laboratory work*, where I also belonged to the team of teachers in the autumn of 2014, we have tried to take every student into account, offering support for those having problems passing the studies. During the spring of 2015, I lectured the course *Molecular modelling* for the last time, but it was still assessed according to the practice of the laboratory.

The courses in Propaedeutic chemistry were never systematically assessed, as the aim of them was to supplement lacks of knowledge in chemistry from pre-university studies. As can be seen in the enclosed teacher portfolio, the courses attracted 50–70 students, which is way over the target group. The courses were found to be fruitful, but they were implemented in the courses of General and Organic chemistry because of overlapping. The courses in Laboratory work were assessed according to the practice of the laboratory.

Compilations of the assessments and student voices (in Swedish) can be seen in the enclosed teacher portfolio.

4) Administration, Positions of Trust and Leadership

- **LEADERSHIP TRAINING**

Åbo Akademi University, Turku, Finland

- Educational leadership, 29 credits (grade 5/5), 31.5.**2018**
- Being head at ÅAU – superior introduction at FSE, 18.11.**2015**

- **POSITIONS OF TRUST**

Åbo Akademi University, Turku, Finland

- Deputy member of the **Department Council of Natural Sciences** **2013–2014**
- Member of the **Department Council of Natural Sciences** **2010–2012**

5) Social Activities

- **EXPERIENCE OF THE UNIVERSITY'S SOCIETAL TASK**

Guest column about grant research in *Meddelanden från Åbo Akademi* **No 3, April 2014**

- **PUBLIC POSITIONS OF TRUST AND MERITS**

Housing company

- Chair of the committee of As Oy Paaskunnanlehto in Turku **2021–Present**

Comprehensive school

- Member of the parents' committee (Hem och skola) of Sirkkala in Turku **2016–2022**
- Member of the parents' committee of S:t Olofsskolan in Turku **2022–Present**

Athletics, PBs; 200 m: 22.82, 400 m: 50.44, 600 m: 1.32.24 (2018, all-time best in M40 in Finland), 800 m: 1.58.21, 1000 m: 2.51.8h (2020, 9th in M40 in Finland), 1500 m: 4.32.32 (2020)

- 16 medals in the Finnish masters athletics championships: 400 m–1500 m **2013–2023**
- Member of the committee of Friidrottsföreningen ÅIFK **2023–Present**
  2017–2020
  1999–2006
- Deputy member of the committee of Friidrottsföreningen ÅIFK **1997–1999**

6) Reference Persons

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