CURRICULUM VITÆ – AATTO LAAKSONEN

Aatto Laaksonen[1,2,3] - Professor (*Em.*) Physical Chemistry

[1] Department of Materials and Environmental Chemistry, Division of Physical Chemistry, Arrhenius Laboratory, Stockholm University (**SU**), 106 91 Stockholm, Sweden
[2] Centre of Advanced Research in Bio-nanoconjugates and Biopolymers, Romanian Academy - Petru Poni (**PP**) Institute of Macromolecular Chemistry, Aleea Grigore Ghica-Voda, 41A, 00487 Iasi, Romania
[3] State Key Laboratory of Materials-Oriented and Chemical Engineering, Nanjing Tech University (**NTU**), Nanjing 210009, China

EDUCATION

1984 **Docent** (Habilitation) – Physical Chemistry **SU**
1981 **PhD** (Fil.Dr.) – Physical/Theoretical Chemistry **SU** Thesis: *Finite Perturbation – Configuration Interaction Calculations of NMR Spin-spin Coupling Constants*
1976 **MSc** (Fil.Kand.) – Mathematics (major) **SU**
1970 **High School & Student Diploma** - Kiukaisten Yhteiskoulu, Kiukainen, Finland

LANGUAGES

Fluent: Swedish, English, Finnish (native)
Passive: German **Beginner:** Italian

WORK EXPERIENCE

Guest Professor (10%) Luleå University of Technology, 2020-
Distinguished Foreign Professor (25%), Nanjing Tech University, Nanjing, China 2019-
Project Director – *5D-nanoP* "Mimicking living matter mechanisms in 5D Chemistry", Iasi, Romania 2018-
Senior Professor - Physical Chemistry (40%), Ångström Laboratory, Uppsala University, 2018

Full Professor - Physical Chemistry (**SU**) 2000- (*Emeritus* 2017-)
Project Leader – *iLEAP* "Ionic liquids for lubrication" (K.A. Wallenberg) 2012-2017
Project Manager – *EXSELENT* "center for porous material" (VR, Vinnova, SU) 2007- 2016
National Expert & Educator in High Performance Computing (HPC-council 50%) 1996-99.
Senior Lecturer - Physical Chemistry (**SU**) 1987 - 1999
Research Associate (**SU**) 1982-86
Teaching assistant (**SU**) 1977-81
First Amanuensis (**SU**) 1976

INTERNATIONAL EXPERIENCE

***STIAS* Fellow**: Stellenbosch Institute of Advanced Study, Stellenbosch South Africa 2014
***KITPC* Fellow**: Kavli Institute of Theoretical Physics, Beijing, China 2013

Visiting Professor

University of Cagliari, Department of Chemistry, Sardinia 2008, 2009, 2011, 2015
Japan Atomic Energy Research Institute (JAERI), Tokai-Mura, Japan 2002, 2005
Dalhousie University, Chemistry Department , Halifax, Canada 1993-94, 1995

Post-doctoral Fellow

IBM Research Laboratories, Kingston, USA 1984-85 (host: Enrico Clementi)
IBM Research Laboratories, Poughkeepsie ,USA 1983 (host: Enrico Clementi)
Daresbury Laboratory, United Kingdom 1982 (host: Victor R Saunders)

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RESEARCH

Multi-scale & multi-granular modeling in Materials & Nano Science,
green molecular chemical engineering and Bio Sciences & Pharma.
Metrix: **300**+ scientific peer-reviewed articles, **20**+ Book chapters.
Google Scholar (Sept 2020): **9350+** citations, H-index = **48**, I10-index = **176**.

CURRENT MAIN FUNDING

1. Swedish Science Council (VR) Project: 2019-03865
In silico studies of multi-responsive polymers as vectors
for drug/gene delivery and controlled release (PI)

2. Swedish Science Council (VR) Project: 2016-04023
Multi-scale modelling of interfacial properties for CO2
separation with deep eutectic ionic liquid-based solvents (co-PI)

3. Swedish Science Council (VR) Project: 2013-04725
Modelling hard, porous, soft and biological materials
- across spatial and temporal scales: from first-principles
to finite elements. (PI)

4. Ministry of Research and Innovation of Romania,
CNCS - UEFISCDI PN-III-P4-IDPCCF-2016-0050,
within PNCDI III. (co-PI & coordinator)
5D-nanoP Mimicking living matter mechanisms by
five-dimensional chemistry approaches

PhD SUPERVISION & EVALUATION

PhD students supervised: **21**. Faculty opponent in PhD defenses **15** times & PhD committee member **25** times in Swedish, Finnish, Norwegian, Belgian, South African, Australian & Irish PhD defenses.
Post-docs supervised: **20**

Current supervision of PhD students and Post docs

PhD student: *Petru Tirnovan, Yunhao Sun, Qingwei Gao* Post-doc: *Hanwen Pei*

Visiting Professors hosted – "Their project" (Their home institute)

Elena Brodskaya "Theory of aqueous surfaces" (St Petersburg State University, Russia)
Francesca Mocci "simulation of Quadrupolar NMR relaxation" (University of Cagliari, Italy)
Peter Kusalik "Nucleation theories" (University of Calgary, Canada)
Zhongyuan Lu "Dissipative Particle Dynamics" (TheoChem State key laboratory, Jilin University
Christopher Jesudason "Polyelectrolyte modelling" (University of Malaya)
Hui Lu "Modelling ZnO" (East China Technical University, Shanghai, China)
Nikolas Benetis "Modelling of molecular radicals" (University of West Macedonia, Greece)

DUTIES IN SCIENTIFIC COMMUNITY

Peer-reviewer to virtually all journals in own field, Book reviews: **2**, Editorial boards: **3**, member in European networks: **7** (in steering board: **3**). Evaluator of grant proposals for Swedish, EU, Irish, Israeli, Belgian & Romanian National Science Councils. Evaluator of HPC resources for Swedish, Danish and Swiss Super-computing centers.
Co-founder and vice-chairman of Theoretical Chemistry section in Swedish Chemical Society.

CONFERENCES

Organization of conferences & workshops: **22**. Invited speaker at conferences: **20** (last 10 years).

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TEACHING

35 years' teaching at all levels of academic education, including General Chemistry, Physical Chemistry, Biophysics, Molecular modelling. Also high school Chemistry for high school students entering Science programs at university. **Author** of notebooks, tutorials, **developer** of theory and laboratory courses.

LECTURING IN WORKSHOPS & SCHOOLS

Winter/Summer Schools & workshops

Summer School in Molecular Modeling, Pula, Sardinia 2019 & 2020. Molecular Modelling, Petru Poni Institute, Iasi, Romania, 2019. Multiscale Modeling, Nanjing Tech University, China 2018. School on Biological Soft Matter, São Paulo, Brazil 2017. III Escola Brasileira de Modelagem Molecular 2015. Molecular modeling, Kosice, Slovakia, 2015. Advanced Molecular Simulation Methods in Physical Sciences, Kavli Institute of Theoretical Physics, Beijing China, 2013. II Escola Brasileira de Modelagem Molecular 2013. Multi-scale modeling, Cagliari (2012), Namur, Belgium (2011), Changchun, China (2010), Singapore (2010). CCP5 Summer school, Bath, UK (2006), SoftSimu2002, Summer graduate school in Helsinki, Finland (2002), Research School in High Performance Computing, Ångström Laboratory, Uppsala (1999), Summer School in Message Passing for MD and MC methods (1996), Summer School in Biocomputing, Royal Institute of Technology, Stockholm (1997), Jyväskylä Summer School in Chemistry, Physics and Mathematics (1992), Graduate School in Laser Spectroscopy, Moscow State University (1992), Winter School in Ultrafast Phenomena, Borgafjäll (1993), Helsinki Winter Schools in Theoretical Chemistry: Solvation Phenomena (1989), Quantum Pharmacology (1991), Solvation Models (1997)

INVITED SPEAKER AT CONFERENCES/WORKSHOPS (SELECTION FROM LAST 10 YEARS)

2020 WATOC World Association of Theoretical and Computational Chemists (moved to 2021), Vancouver
2020 New Trends in Macromolecular and Supra Molecular Chemistry (moved to 2021), Iasi, Romania
2019 Scientific Summer School in Molecular Modeling: Real Applications and New Approaches, Pula, Sardinia
2019 From Atomistic to Subatomistic Computational Simulations, Namur, Belgium
2018 CECAM Workshop, Coupling and Linking Simulations, Lausanne, Switzerland
2018 Essence/EMMC Physics vs Data based modelling, Uppsala, Sweden
2018 International Workshop on Soft Matter & Biophysics Theories, Beijing, China
2017 Center of Molecular Simulation Invited Seminar Series, Calgary, Canada
2017 Colloquium IFT/ICTP-SAIFR Colloquium São Paulo, Brazil
2015 PacifiChem, Honolulu, Hawaii
2015 TheoBio2015, Cagliari, Italy.
2015 Modeling &Simulation of Biological/Macromolecular Systems, Changchun, China
2015 Korea-Sweden Excellence Seminar, Seoul, Korea
2014 Multi-scale Simulation Methods for Soft Matter Systems, Mainz, Germany
2014 The eSSENCE Multi-scale Materials Modelling, Uppsala, Sweden
2013 Intermolecular Interactions in Crystals via Experiment and Theory**, Pula**, Sardinia
2012 International Society of Quantum Biology and Pharmacology President's Meeting: Stockholm,
2012 Annual International Conference on Systems Biology (ICCSB2012), Shanghai, China (*keynote*)
2011 WATOC World Association of Theoretical and Computational Chemists Santiago del Campostela, Spain

Contributions to careers of excellent young researchers

Every one of my 21 former PhD students and 20 post-docs have made a successful career. The majority of them are now university professors (full, associate or assistant), many have good research positions in solid companies and many are entrepreneurs including founders/CEOs of biopharma companies.

MAJOR SOFTWARE DEVELOPMENTS

1. A Coupled Hatree-Fock (CHF) *ab initio* perturbation theory program for NMR J-couplings*)
2. A Spin-unrestricted Multi-Configurational SCF quantum chemistry software**)
3. McMoldyn: Simulation package for liquids & solids *(Comp.Phys.Commun.*, 1986, **42**, 271.
4. M.Dyna*Mix* - a scalable portable parallel MD simulation package *(Comp.Phys.Commun.*, 2000, **128**, 565.

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5. gOpenMol – visualisation software (J. Molec. Graph. & Model. 1998, 15, 301)
*)Developed in my PhD thesis **)To compute J-couplings for triplet unstable molecules

WORKING EXPERIENCE OUTSIDE ACADEMY

Lease of a tourist area with a campsite and cottages in Padasjoki, Finland and its operation (1970).
Owner of a two-floor quarter restaurant and a hamburger bar in Tampere, Finland (1970-1972).
Younger cook at the restaurant/night club *Ikituuri*, Turku, Finland (1972).
Nurse (Summer substitute) at Beckomberga mental hospital, Stockholm (1973,1974,1975 & 1976)

OWN ENTREPRENEURSHIP

Did register a consulting company BIO4CAST in Computer Modeling of Scientific Problems and data analysis after won the first prize for the best commercialization idea in the first edition of the Swedish Royal Academy of Engineering Mentor4Reseach competition (2006). The prize money 10000 euro was used to start the company. The company is currently on hold.

HOBBIES

Everything connected to Nature and how it can be experienced
Traveling and exploring new countries, societies and cultures
Music, theater, exhibitions, movies
Food, wine and friendly & funny people around them.