CURRICULUM VITAE

Personal information

Name, Surname:	Aatto Ilmari Laaksonen		
Date of birth:	[redacted]	Gender:	Male
Nationality:	Swedish and Finnish		
Researcher unique identifier(s) (ORCID, Researcher ID etc.):	ORCID 0000-0001-9783-4535, UEF-ID / BrainMap ID 82884611		
Personal link from the platform at https://www.brainmap.ro/	https://www.brainmap.ro/aatto-laaksonen		
URL for personal website (if case):	https://www.su.se/english/profiles/a/aatto		

Education

Year	Faculty/department - University/institution - Country
1984	Habilitation (Docent) in Physical Chemistry – Stockholm University, Sweden
1981	PhD (Fil.Dr.) in Physical/Theoretical Chemistry – Stockholm University, Sweden. Thesis: Finite Perturbation–Configuration Interaction Calculations of NMR Spin–Spin Coupling Constants.
1977–1979	Studies in Computer Science – Royal Institute of Technology (KTH), Sweden
1976	MSc (Fil.Kand.), Mathematics major – Stockholm University, Sweden

Positions - current and previous

(*Academic sector/research institutes/industrial sector/public sector/other)*

Year	Job title – Employer – Country
2023–present	Guest Professor, WISE/Creaternity – Luleå University of Technology, Sweden
2022–2027	Horizon Europe ERA Chair, BioMat4CAST – "Petru Poni" Institute of Macromolecular Chemistry (ICMPP), Romanian Academy, Iaşi, Romania
2019–present	Distinguished Foreign Professor – Nanjing Tech University, China
2000–2017, 2017– present	Professor of Physical Chemistry, Professor Emeritus – Stockholm University, Sweden
2018–2019	Senior Professor of Physical Chemistry – Ångström Laboratory, Uppsala University, Sweden
1987–1999	Senior Lecturer in Physical Chemistry – Stockholm University, Sweden
1982–1986	Research Associate – Stockholm University, Sweden
1982–1985	Postdoctoral Fellow / Research Associate – SERC Daresbury Laboratory, UK, and IBM Research Laboratories, USA
1976–1981	First Amanuensis / Teaching Assistant – Stockholm University, Sweden

Project management experience

Year	Project title - Role – Funder – Budget – link to project webpage
2022–2027	BioMat4CAST, "Petru Poni Institute Multi-scale In Silico Laboratory for Complex and Smart Biomaterials" (ID 101086667) – ERA Chair / Scientific Leader – Horizon Europe – EUR 2.5 M – https://cordis.europa.eu/project/id/101086667
2018–2022	5D-nanoP, "Mimicking living matter mechanisms by five-dimensional chemistry approaches" (PN-III-P4-ID-PCCF-2016-0050) – Project Coordinator – UEFISCDI – appr. EUR 1.5 M

2022–2027	Linked Kempe projects on ionic-liquid/NADES biomass processing and green H2 production (SMK21-0011, SMK24-0137) – Principal Investigator – Kempe Foundations – appr. EUR 250 k
2021–2024	“Multiscale studies of aqueous neoteric liquids – ionic liquids and deep eutectic solvents” (2020-03899) – Co-PI – Swedish Research Council – appr. EUR 360 k
2020–2023	“In silico studies of multi-responsive polymers as vectors for drug/gene delivery and controlled release” (2019-03865) – Principal Investigator – Swedish Research Council – appr. EUR 340 k
2012–2017	iLEAP, “Ionic liquids for lubrication” – Project Leader for computational research – Knut and Alice Wallenberg Foundation
2007–2016	EXSELENT Centre for Porous Materials – Project Manager / computational research lead – Swedish Research Council, Vinnova and Stockholm University

Other relevant professional experiences

Year	Description - Role
1986-2026	Mentoring and academic leadership: Supervised 25 PhD students and 20 postdoctoral fellows, hosted 7 visiting professors, served as faculty opponent in 15 PhD defences and member of 25 doctoral examination committees across seven countries
1977-2005	Method and software development: Developed or co-developed Coupled Hartree–Fock and spinunrestricted MCSCF codes, McMoldyn, M.DynaMix and gOpenMol, together with Inverse Monte Carlo coarse-graining, Expanded Ensemble free-energy methods, QM/MM coupling schemes, NlogN Ewald summation and cross-grained elastic-network models
1993-2018 2000-2018	International recognition and service: KITPC Fellow (2013), STIAS Fellow (2014), visiting professor/scientist in Italy, Japan, Canada, Singapore, Brazil, China, Slovakia and Belgium. Evaluator for Swedish, EU, Irish, Israeli, Belgian and Romanian funding bodies and several European supercomputing centres
2000-2023 1987-2018	Editorial, professional and educational roles: Editor of Comprehensive Computational Chemistry (Elsevier, 2023) and Advances in Algorithms for Macromolecular Simulations (Springer, 2003), editorial board service, co-founder and former vice-chair of the Theoretical Chemistry Section of the Swedish Chemical Society, more than 35 years of university teaching and advanced international summer-school teaching.
2006	Innovation award. First prize, “Best business idea from academia”, Royal Swedish Academy of Engineering Sciences (IVA)

Track record of the last 10 years

1. Ma, C., Laaksonen, A., Liu, C., Lu, X., Ji, X. “The Peculiar Effect of Water on Ionic Liquids and Deep Eutectic Solvents.” Chemical Society Reviews 47 (2018) 8685–8720. DOI: 10.1039/C8CS00325D. Contribution: Established a molecular framework for understanding water-controlled structure and properties in IL/DES systems.

2. Wang, Y.-L., Li, B., Sarman, S., Mocci, F., Lu, Z.-Y., Yuan, J., Laaksonen, A., Fayer, M. D. “Microstructural and Dynamical Heterogeneities in Ionic Liquids.” Chemical Reviews 120 (2020) 5798–5877. Contribution: Synthesized the multiscale physical picture of ionic-liquid heterogeneity and dynamics.

3. Mocci, F. et al. “Carbon Nanodots from in Silico Perspective.” Chemical Reviews 122 (2022) 13709–13799. DOI: 10.1021/acs.chemrev.1c00864. Contribution: Demonstrated the integration of electronicstructure, atomistic and mesoscale modelling for complex nanomaterials.

4. Lyubartsev, A. P., Laaksonen, A. “Hierarchical Multiscale Modeling Through Inverse Problem Solving.” In Comprehensive Computational Chemistry, Elsevier (2023). DOI: 10.1016/B978-0-12-821978-2.00121-5. Contribution: Consolidated the inverse-problem strategy that underpins the proposed multiscale methodology.

5. Neamtu, A. et al. “Molecular dynamics simulations reveal the hidden EF-hand of EF-SAM as a possible key thermal sensor for STIM1 activation by temperature.” Journal of Biological Chemistry 299 (2023) 104970. DOI: 10.1016/j.jbc.2023.104970. Contribution: Connected atomistic simulation with a testable biomolecular mechanism.

6. An, R. et al. “Integrative studies of ionic liquid interface layers: bridging experiments, theoretical models and simulations.” Nanoscale Horizons 9 (2024) 506–520. DOI: 10.1039/D4NH00007B. Contribution: Advanced experiment–simulation integration for ionic-liquid interfaces.

7. de Villiers Engelbrecht, L., Cibotariu, N., Ji, X., Laaksonen, A., Mocci, F. “Deep Eutectic Solvents Meet Non-Aqueous Cosolvents: A Modeling and Simulation Perspective.” Journal of Chemical & Engineering Data 70 (2025) 19–43. DOI: 10.1021/acs.jced.4c00505. Contribution: Provided transferable modelling principles for multicomponent DES formulations.

8. Puf, R., Fundueanu, G., Constantin, M., Ferariu, A., Laaksonen, A. “Beyond poly(NIPAAm): Molecularly engineered biodegradable pullulan microgels with excellent thermosensitivity. Design, modeling, and realization.” Chemical Engineering Journal 523 (2025) 167673. DOI: 10.1016/j.cej.2025.167673. Contribution: Integrated molecular design, modelling and experimental realization of a responsive biomaterial.

9. Murnikova, Ž. et al. “On the mechanism behind the enhanced solubility of glibenclamide in aqueous ionic liquid solution.” Journal of Molecular Liquids 422 (2025) 127153. DOI: 10.1016/j.molliq.2025.127153. Contribution: Resolved a pharmaceutical-solvation mechanism in an aqueous ionic-liquid system.

10. Perepelytsya, S. et al. “Ions as Architects of DNA Nanostructures: Mechanisms, Simulations, and Technological Frontiers.” Small Structures (2026), in press. DOI: 10.1002/sstr.202500786. Contribution: Summarized ion-mediated nucleic-acid structure and its implications for delivery and nanotechnology.

Narrative CV

A narrative summarizing which work has had the greatest importance and impact.

Scientific trajectory and independent contributions. My scientific career has followed a continuous movement from mathematics and computer science to theoretical chemistry, molecular simulation, biomolecular science and materials engineering. During my PhD I developed a 25,000-line Coupled Hartree– Fock program for NMR spin–spin coupling constants. At SERC Daresbury Laboratory I created a spinunrestricted multiconfigurational SCF implementation, and at IBM Research I moved into molecular dynamics, parallel computing, nucleic-acid modelling and ion-channel simulations. Returning to Sweden, I helped establish molecular simulation as an independent research activity and built a group combining method development with close experimental validation

Methods that changed research practice. My most lasting contributions are methodological. I introduced long-range Ewald electrostatics into early explicit-solvent biomolecular simulations, developed highly parallel linked-cell algorithms, contributed to QM/MM coupling, absolute free-energy and chemical-potential calculations through the Expanded Ensemble method, and co-developed the M.DynaMix and gOpenMol

software environments. With Alexander Lyubartsev I introduced the Inverse Monte Carlo method for deriving effective coarse-grained interactions from structural data. This inverse-problem philosophy anticipated modern multiscale modelling and remains central to connecting molecular detail with experimentally accessible length and time scales
Interdisciplinary reach and recent scientific focus. I have applied these methods to nucleic acids, proteins, membranes and ion channels, drug design and transport, solvation, carbohydrates, atmospheric processes, porous materials, tribology and responsive polymers. During the last fifteen years, ionic liquids and deep eutectic solvents have become a major focus, with more than 50 publications spanning bulk liquids, water and cosolvent effects, interfaces, confinement, lubrication, biomass processing, energy and pharmaceutical solvation. Recent work increasingly links molecular modelling with experiments, machine learning and digitaltwin concepts, rather than treating simulation as a stand-alone descriptive tool
Leadership and capacity building in Romania. I have already led two major initiatives at the “Petru Poni” Institute. As Coordinator of the UEFISCDI 5D-nanoP project, I integrated in silico design, supramolecular chemistry, responsive polymers and biomedical validation across a large multidisciplinary team. As ERA Chair of BioMat4CAST, I am now building a sustainable multiscale computational-chemistry capability at ICMPP, recruiting and mentoring young researchers and connecting the institute to international modelling, biomaterials and AI networks. These roles demonstrate both scientific leadership and the practical ability to implement complex projects in the Romanian research environment.
Mentoring and research culture. I have supervised 25 PhD students and 20 postdoctoral fellows and have trained researchers from chemistry, physics, materials science, chemical engineering and biomedicine. My mentoring approach is to give young researchers ownership of a scientifically meaningful problem while providing rigorous training in physical reasoning, reproducibility, software, uncertainty and communication. Many of my projects have deliberately paired modellers with experimentalists so that each side learns the constraints and strengths of the other.