Curriculum Vitae

Hilda Sandström

E-mail: hilda.sandstrom@aalto.fi
Webpage: https://hilsan.github.io/
Github/Gitlab: https://github.com/hilsan | https://gitlab.com/hilsan
Social: ResearchGate, LinkedIn, ORCID, Web of Science

Expertise

Cheminformatics – Computational chemistry – Molecular and atmospheric modeling – Machine learning for chemical systems – Structure and property prediction – Multiscale simulation methods – Environmental data analysis

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Education and Employment

Postdoctoral Researcher, Machine learning for Atmospheric Chemistry

Computational modelling of atmospheric compounds and mass spectrometry
Aalto University, Espoo, Finland (25/09/2022 – current)

- Investigated the overlap between atmospheric compounds and the molecules found in mass spectral libraries.
- Co-developed a new cheminformatics descriptor.
- Co-created a model for predicting chemical ionization mass spectrometry peak intensities.
  Supervisor: Prof. Patrick Rinke

Research visit, Atmospheric chemistry lab

- University of Gothenburg (GU), Sweden
- September 2024–current
- Description: Machine learning applications to experimental atmospheric chemistry data.
  Mentor: Prof. Mattias Hallqvist

Doctorate Degree in Theoretical Chemistry

Chalmers University of Technology, Sweden
(Degree issued: 02/06/2022)

- Thesis title: Nitriles in Prebiotic Chemistry and Astrobiology
- Focus: Examined the role of hydrogen cyanide and hydrogen cyanide polymers in astrochemistry and astrobiology using computational chemistry and ab initio molecular dynamics.
  Thesis advisor: Prof. Martin Rahm

MEng in Chemical Engineering with Engineering Physics

Chalmers University of Technology, Sweden
(Degree issued: 08/11/2017)

- Thesis title: Understanding the Mechanism of PAQR-2 Through Modeling and Simulations
- Investigated the effects of rigid and fluid membranes on protein conformation by molecular dynamics simulations with classical force fields.
  Thesis advisor: Dr. Samuel Genheden (University of Gothenburg)

Peer-Reviewed Scientific Publications

(Google Scholar, 28/05/2025)

Total citations: 89, h-index: 5 , i-index: 4

1. Sandström, H., & Rinke, P. *Geoscientific Model Development*, 18, 2701–2724 (2025). DOI: 10.5194/gmd-18-2701-2025
2. Malaska, M. J., et al., *Astrobiology*, 25 (2025). [I performed geometry optimizations and molecular measurements and student supervision.]
3. Bortolussi, F. et al., *Atmospheric Chemistry and Physics*, 25, 685-704 (2025). DOI: 10.5194/acp-25-685-2025. [I helped design study, supervised, and contributed to programming and model testing.]
4. Sandström, H., et al., *ACS Earth and Space Chemistry*, 8, 1272–1280 (2024). DOI: 10.1021/acsearthspacechem.4c00088.
5. Sandström, H., et al., *Advanced Science*, 11, 2306235 (2024). DOI: 10.1002/advs.202306235.
6. Sandström, H., & Rahm, M., *The Journal of Physical Chemistry A*, 127, 4503–4510 (2023). DOI: 10.1021/acs.jpca.3c01504.
7. Sandström, H., & Rahm, M., *ACS Earth and Space Chemistry*, 5, 2152–2159 (2021). DOI: 10.1021/acsearthspacechem.1c00195.
8. Sandström, H., & Rahm, M., *Science Advances*, 6, eaax0272 (2020). DOI: 10.1126/sciadv.aax0272.
9. Lindblom, A., et al., *Diagnostic Microbiology and Infectious Disease*, 93, 380–385 (2019). DOI: 10.1016/j.diagmicrobio.2018.10.014
   [I performed fluorescence microscopy assays where I stained, trapped, and photographed plasmids in nanochannels.]

Skills and Competences

Cheminformatics: OpenBabel, RDKit

Electronic structure and thermochemistry codes: VASP, Gaussian, Orca, PHONOPY

Molecular dynamics: CP2K, Gromacs, PLUMED, xTB, VMD (visualization)

Structure prediction and conformational sampling: CALYPSO, CREST

Machine learning: Scikit-learn (proficient), Tensorflow (basic). Graduate-level courses on Artificial Neural Networks and Stochastic Optimization Algorithms (Chalmers University of Technology, 2016)

Programming languages and tools: Python, Atomistic Simulation Environment (ASE), Bash, MATLAB, introductory Java.

Experimental techniques: Fluorescence microscopy, microfluidics for DNA sequence imaging

Languages: Fluent: Swedish (native), English; Intermediate: Italian

Grants, Awards and Fellowships

Marie Skłodowska-Curie Postdoctoral Fellowship (2025)
Awarded by: European Commission, Horizon Europe Programme
Project: CLOUDMAP – Improving atmospheric compound identification with data-driven methods
Host Institution: Technical University of Munich (TUM), Germany
Duration: 24 months (scheduled Oct 2025 – Sep 2027)

LUMI Extreme Scale Access Resource Allocation
Granted by: CSC – IT Center for Science, Finland

Duration: 2024–2025
Project: Advanced modeling of atmospheric compounds using HPC
Details: Allocation awarded on Europe's flagship LUMI supercomputer as part of a competitive application process.

Travel Grants

Nils Philblad's Foundation – 17,000 SEK (2021)

Nils Philblad's Foundation – 3,650 SEK (2019)

Karl and Annie Leon's Foundation – 3,850 SEK (2018)

Teaching Experience

Supervision

Current: Supervising 2 PhD students and 1 undergraduate at Aalto University

Previous: Supervised 4 visiting undergraduates and 12 bachelor's students at Chalmers University of Technology

Teaching Assistant Roles

2017–2021 (Chalmers University of Technology):

Quantum Engineering (MSc): Molecular orbital theory and computational labs

Physical Chemistry (BSc): Quantum chemistry, statistical thermodynamics, spectroscopy, and kinetics

Physical Chemistry (BSc): Kinetics and experimental lab instructor

Theoretical Chemistry (BSc): Quantum chemistry and computational lab instructor

Chemistry and Biochemistry (BSc): Organic synthesis and experimental lab instructor

Calculus (2014): Mathematics tutor

Conference presentations and organization

Presentations

2025 Nordic Workshop on AI for Climate Change (Gothenburg, Sweden) – Machine learning for Atmospheric Mass Spectrometry (Oral)

EGU General Assembly 2025 (Vienna, Austria) – Towards Atmospheric Compound Identification: A Reference Library of Simulated Electron Ionization Mass Spectra (Poster)

2024 European Aerosol Conference (Tampere, Finland) – Advancing property prediction for atmospheric molecules with molecular fingerprints (Poster)

2023 International Aerosol Modeling Algorithms Conference (Remote, USA) - Characterizing Atmospheric Molecules for Machine Learning (Oral)

European Aerosol Conference (Málaga, Spain) - Characterizing Atmospheric Molecules for Machine Learning (Oral)

Physics Days (Tampere, Finland) - Characterizing Atmospheric Molecules for Machine Learning (Oral)

2022 AbSciCon (Atlanta, USA) – Untangling Hydrogen Cyanide Polymerization Using Quantum Chemistry (Oral)

2019 CECAM Workshop (Paris, France) – Quantum Chemical Evaluation of Polarity-Inverted Membranes and Polymers on Titan (Poster)

Astrochemistry Symposium (Gothenburg, Sweden) – Quantum Chemical Evaluation of Polarity-Inverted Membranes and Polymers on Titan (Poster)

2018 National Meeting of the Swedish Chemical Society (Lund, Sweden, Poster)

Organization

2023 ESTML (Levi, Finland) – Session chair for "EST (electronic structure theory) development" and "Software II"

2022 AbSciCon (Atlanta, USA) – Session chair for "From Prebiotic Chemistry to Astrobiology"

Outreach

Climate AI Nordics Network – Core Member, Organizer, and Finland Representative (2025 – present)
Actively contributing to network activities focused on advancing collaboration and research on AI for climate science in the Nordic region.

FysKemDagarna (Physics and Chemistry Days) 2024 – Presenter and panelist on AI in chemistry, physics, and education. Organized by Finnish Society of Chemists (FKS), Finnish Physical Society (FSF), in collaboration with the Chemical Society of Åbo (KSÅ) and Skolresurs.

Participated as a presenter and panelist in discussions on the application of AI in chemistry, physics, and education, engaging an audience of students and high school teachers to promote the integration of AI in science and science education.

Shaking up Tech 2023 – Workshop Organizer. Organized by Aalto University.

Organized and facilitated sessions for the "Molecular AI Laboratory" to inspire women and non-binary individuals to pursue careers in technology and engineering fields.