CV

Hilda Sandström

Nationality – Swedish

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

Expertise

Cheminformatics – Computational chemistry – Advanced molecular dynamics – Molecular modelling – Structure prediction – Machine learning for molecular sciences

Software, modeling and languages

Cheminformatics – OpenBabel, RDKit
Electronic structure/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 & Tensorflow
Programming languages and tools – Python, Atomistic Simulation Environment (ASE), Bash, MATLAB, introductory Java
Languages – Swedish (native), English; Intermediate: Italian

Education and Career

Postdoctoral Researcher (25/09/2022 – current)
Aalto University, Finland

Research focuses on computational modelling for compound identification with mass spectrometry. Developed unsupervised learning approach to estimate molecular similarity of compound classes. Co-developed a new cheminformatics descriptor. Co-created a model for prediction of chemical ionization mass spectrometry peak intensities.

Doctorate Degree in Theoretical Chemistry
Chalmers University of Technology, Sweden
(Degree issued: 02/06/2022)

Thesis title: Nitriles in Prebiotic Chemistry and Astrobiology
Applied quantum chemistry and molecular dynamics methods to examined the formation and stability of polymers relevant to astrochemistry.

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
Applied classic force fields and molecular dynamics to investigate the effects of rigid and fluid membranes on protein conformation.

Peer-reviewed scientific publications

(Google Scholar, 25/08/2025, 12 publications, 6 first author)
Total citations: 93, h-index: 5 , i-index: 4

12. J. Brean, F. Bortolussi, A. Rowell, D. C. S. Beddows, K. Weinhold, P. Mettke, M. Merkel, A. Kumar, S. Barua, S. Iyer, A. Karppinen, **Sandström, H.**, P. Rinke, A. Wiedensohler, M. Pöhlker, M. Dal Maso, M. Rissanen, Z. Shi, & R. M. Harrison, *ACS ES&T Air*, 2, 1704–1713 (2025). DOI: 10.1021/acsestair.5c00119 [Supervised PhD student F. Bortolussi in developing and evaluating the machine learning model
11. F. Izquierdo-Ruiz, M. L. Cable, R. Hodyss, T. H. Vu, **Sandström, H.**, A. Lobato, & M. Rahm, *Proc. Natl. Acad. Sci. U.S.A.*, 122, e2507522122 (2025). DOI: 10.1073/pnas.2507522122 [Developed and tested crystal structure prediction program workflow for molecular cocrystals of hydrogen cyanide.]
10. R. R. Valiev, R. T. Nasibullin, **Sandström, H.**, P. Rinke, K. Puolamäki, & T. Kurten, *Physical Chemistry Chemical Physics*, 27, 14804–14814 (2025). DOI: 10.1039/D5CP01101A[Co-advisor for ML workflow; developed MBTR model.]
9. Bortolussi, F., **Sandström, H.**, F. Partovi, J. Mikkilä, P. Rinke, & M. Rissanen, *Atmospheric Chemistry and Physics*, 25, 685–704 (2025). DOI: 10.5194/acp-25-685-2025 [Co-designed study, supervised, and contributed to programming and model testing.]
8. Malaska, M. J., **Sandström, H.**, A. E. Hofmann, R. Hodyss, L. Rensmo, M. van der Meulen, M. Rahm, M. L. Cable, & J. I. Lunine, *Astrobiology*, 25 (2025). DOI: 10.1089/ast.2024.0125 [Performed geometry optimizations and molecular measurements and student supervision.]
7. **Sandström, H.**, P. Rinke, *Geoscientific Model Development*, 18, 2701–2724 (2025). DOI: 10.5194/gmd-18-2701-2025
6. **Sandström, H.**, M. Rissanen, J. Rousu, P. Rinke, *Advanced Science*, 11, 2306235 (2024). DOI: 10.1002/advs.202306235
5. **Sandström, H.**, F. Izquierdo-Ruiz, M. Cappelletti, R. Dogan, S. Sharma, C. Bailey, & M. Rahm, *ACS Earth and Space Chemistry*, 8, 1272–1280 (2024). DOI: 10.1021/acsearthspacechem.4c00088
4. **Sandström, H.**, & Rahm, M., *The Journal of Physical Chemistry A*, 127, 4503–4510 (2023). DOI: 10.1021/acs.jpca.3c01504
3. **Sandström, H.**, & Rahm, M., *ACS Earth and Space Chemistry*, 5, 2152–2159 (2021). DOI: 10.1021/acsearthspacechem.1c00195
2. **Sandström, H.**, & Rahm, M., *Science Advances*, 6, eaax0272 (2020). DOI: 10.1126/sciadv.aax0272
1. Lindblom, A., K. K. Sriram, V. Müller, R. Öz, **Sandström, H.**, C. Åhrén, F. Westerlund, & N. Karami, *Diagnostic Microbiology and Infectious Disease*, 93, 380–385 (2019). DOI: 10.1016/j.diagmicrobio.2018.10.014 [Performed fluorescence microscopy assays where I stained, trapped, and photographed plasmids in nanochannels.]

Teaching experience

Supervision

2022-2025 Aalto
Supervisor of 2 PhD students and 1 undergraduate at Aalto University

2018-2022 *Chalmers*
Supervisor of 4 visiting and 12 bachelor's students

Teaching Assistant Roles

2017–2021 Chalmers
Quantum Engineering (MSc)
Physical Chemistry (BSc)
Physical Chemistry (BSc)
Theoretical Chemistry (BSc)
Chemistry and Biochemistry (BSc)

Grants, awards and fellowships

Marie Skłodowska-Curie Postdoctoral Fellowship (2025)
Awarded by the European Commission, Horizon Europe Programme

LUMI Extreme Scale Access Resource Allocation (2024)
Awarded by CSC IT Center for Science, Finland

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)

Conference presentations, organization and outreach: Highlights

Presentations

2025 *Nordic workshop on AI for climate change* (Sweden) – Machine learning for atmospheric mass spectrometry (Oral)

2023 *International aerosol modeling algorithms conference* (USA) – Characterizing Atmospheric Molecules for Machine Learning (Oral)
European aerosol conference (Spain) – Characterizing Atmospheric Molecules for Machine Learning (Oral)
Physics days (Finland) – Characterizing atmospheric molecules for machine learning (Oral)

2022 *AbSciCon* (USA) – Untangling hydrogen cyanide polymerization using quantum chemistry (Oral)

Organization

2025 Nordic workshop on AI for climate change (Sweden)

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

2025 *Climate AI nordics network* – Core member and organizer. Finland representative.

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

2023 *Shaking Up Tech 2023* –Workshop organizer at Aalto University.