CURRICULUM VITAE

HILDA SANDSTRÖM

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CORE COMPETENCES

- Scientific leadership
- Project management
- Molecular modelling & simulation
- Structure prediction
- Cheminformatics
- Machine learning for chemistry
- High-performance computing (HPC)
- Student supervision & mentoring
- Interdisciplinary collaboration
- Scientific communication

PROFESSIONAL AND ACADEMIC CAREER

Since 10/2025	**Marie Skłodowska-Curie postdoctoral researcher** *Technical University of Munich, Germany* Main project Machine learning–based compound identification with mass spectrometry ▪ Developed machine learning models for mass spectrometry signal prediction and dataset similarity analysis. ▪ Develop protocols for simulating mass spectrometry data for atmospheric compounds ▪ Coordinated interdisciplinary projects and supervised students.
9/2022 – 9/2025	**Postdoctoral researcher** *Aalto University, Finland* Main project Machine learning–based compound identification with mass spectrometry ▪ Developed machine learning models for mass spectrometry signal prediction and dataset similarity analysis. ▪ Designed molecular descriptors enabling interpretable machine learning models. ▪ Benchmarked models and descriptors for reaction rate prediction. ▪ Coordinated interdisciplinary projects and supervised students.
9/2017 – 5/2022	**Early-stage researcher (PhD)** *Chalmers University of Technology, Sweden* Main project Kinetic modeling and molecular structure prediction in polymerization reactions ▪ Applied steered molecular dynamics, density functional theory, umbrella sampling, and metadynamics for reaction pathway exploration and free-energy profiling. ▪ Predicted crystal structures of molecular co-crystals and identified plausible reaction products from kinetics/thermodynamics. ▪ Coordinated multi-site collaborations on crystal structure prediction and lipid conformer analysis; advised students.
9/2024 – 9/2025	**Visiting postdoctoral researcher** *University of Gothenburg, Sweden* Simulated mass spectrometry signals using machine learning models, molecular dynamics, reaction exploration and quantum chemistry

ACADEMIC STUDIES

9/2017 – 5/2022	**PhD** in Chemistry (Theoretical chemistry) *Chalmers University of Technology, Sweden.* **Award date** 02/06/2022. Thesis – *Nitriles in Prebiotic Chemistry and Astrobiology* Supervisor – Prof Martin Rahm.
8/2012 – 9/2017	**MEng** in Chemical engineering with engineering physics *Chalmers University of Technology, Sweden.* **Award date** 08/11/2017. Thesis – *Understanding the Mechanism of PAQR-2 Through Modeling and Simulations* *Supervisor – Dr. Samuel Genheden.*
8/2015 – 9/2017	**MSc** in Engineering physics (Nanotechnology master program, integrated) *Chalmers University of Technology, Sweden.* **Award date** 08/11/2017.
8/2012 – 6/2015	**BSc** in Chemical engineering with engineering physics (integrated) *Chalmers University of Technology, Sweden.* **Award date** 12/06/2015.

SOFTWARE AND MODELING SKILLS

Programming: Python, MATLAB, Bash – Well Experienced | **Machine Learning and Cheminformatics:** Scikit-learn, TensorFlow, RDKit, OpenBabel, ASE – Experienced | **Molecular Dynamics and Simulation:** CP2K, GROMACS, PLUMED – Expert; xTB, QCxMS, VMD – Experienced | **High-Performance Computing (HPC):** Parallel computing, cluster resource management – Experienced | **Version Control:** Git –Experienced

PEER-REVIEWED SCIENTIFIC PUBLICATIONS

(Google Scholar, 24/11/2025, 13 peer-reviewed articles, 6 first author)
Total citations: 110, h-index: 5 , i-index: 4

13. Madan, I., Aliabadi, S. A., Huhtasaari, J., Matic, E., Hogedal, E., Kamińska, K., Nilsson, F., Stark, A., Izquierdo-Ruiz, F., **Sandström, H.**, Rahm, M.*QRB Discovery*, 6, e23 (2025). DOI: 10.1017/qrd.2025.10012 [Supervised students and co-created workflow for testing stability of polymers.]
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 and workflow]
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]
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, advised, 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, conformer search 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, PEDAGOGICAL EXPERIENCE AND SUPERVISION OF STUDENTS

LECTURES AND EXERCISES

Year	Subject	Degree	Type	Week hours
2018 – 2020	Quantum engineering	1st year MSc Nanotechnology	Computer labs	2
2018 – 2021	Physical chemistry	2nd year BSc Biotechnology	Tutorials and experimental labs	12
2018 – 2021	Theoretical chemistry	3rd year Bsc Chemical engineering with engineering physics	Computer labs	4
2017 – 2018	Chemistry and biochemistry	1st year BSc Chemical engineering	Experimental labs	8
2014	Calculus	1st year BSc Chemical engineering with engineering physics	Exercise	1

PEDAGOGICAL TRAINING

2019	Teaching, learning and evaluation at Chalmers University of Technology (3 ECTS)

SUPERVISION OF STUDENTS

Since 2024	Supervisor of MSc student at Aalto University
Since 2024	Advisor of PhD student at Aalto University
Since 2022	Co-supervisor of PhD student at University of Helsinki
11/2024 – 5/2024	Supervisor of BSc student at Aalto University
5/2021 – 9/2021	Co-supervisor of 2 visiting and 3 BSc students at Chalmers University of Technology
1/2021 – 6/2021	Co-supervisor of 6 BSc students at Chalmers University of technology
6/2020 – 8/2020	Supervisor of 2 BSc students at Chalmers University of Technology
1/2020 – 6/2020	Supervisor of 6 BSc students at Chalmers University of Technology
4/2019 – 7/2019	Supervisor of visiting BSc students at Chalmers University of Technology
4/2018 – 6/2018	Supervisor of one BSc student at Chalmers University of Technology

FUNDING AND RESOURCE ACQUISITIONS

2025	202k EUR Marie Skłodowska-Curie postdoctoral fellowship
2024 – 2025	LUMI extreme scale access resource allocation
2018 – 2021	Selected travel grants: Nils Philblad Foundation (2021), Karl and Annie Leon's Foundation (2018–2019)

CONFERENCE CONTRIBUTIONS

2025	**Keynote** Atmospheric day, Sweden. CLOUDMAP – *Advanced identification of atmospheric compounds*
2025	**Invited talk** Nordic Workshop on AI for Climate Change, Sweden. *Machine learning for atmospheric mass spectrometry*
2024	**Invited talk** FysKemDagarna (Physics and Chemistry Days), Sweden. *AI in Chemistry: Solving experimental challenges with artificial intelligence*
2023	International Aerosol Modeling Algorithms Conference, USA. *Characterizing Atmospheric Molecules for Machine Learning*
2023	European Aerosol Conference, Spain. *Characterizing Atmospheric Molecules for Machine Learning*
2023	Physics Days, Finland. *Characterizing atmospheric molecules for machine learning*
2022	AbSciCon, USA. *Untangling hydrogen cyanide polymerization using quantum chemistry*

ACADEMIC SERVICES

2025	Reviewer for *ACS Earth Space Chem, ACS Omega* and *Atmospheric Chemistry and Physics*.
2025	Organizing committee. *Nordic Workshop on AI for Climate Change*, Sweden.
2025	Core member, organizer and Finland representative. *Climate AI Nordics Network.*
2024	Panelist on AI in chemistry, physics, and education, *FysKemDagarna (Physics and Chemistry Days).*
2023	Organizer of workshop hands-on session. *Shaking Up Tech 2013.* Workshop for underrepresented groups in STEM, Aalto University, Finland.
2023	Session chair and organizer. *ESTML*, Levi, Finland.
2022	Session chair. *AbSciCon*, USA.

LANGUAGES

Swedish (Excellent) | English (Excellent) | Italian (Intermediate) | French (Basic)