CV

GENERAL INFORMATION

Name	Hilda Sandström
Position	Marie Skłodowska-Curie postdoctoral researcher
Institution	Technical University of Munich, Germany
Email	hilda.sandstroem@tum.de
ORCID	0000-0001-7845-1088
Google Scholar	scholar.google.com

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

EXPERIENCE

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.

9/2024 – 9/2025 — **Visiting postdoctoral researcher**
University of Gothenburg, Sweden
Simulated mass spectrometry signals using machine learning models, molecular dynamics, reaction exploration and quantum chemistry.

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.

EDUCATION

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.

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.

TEACHING

LECTURES AND EXERCISES

2018–2020 — **Quantum engineering**
Chalmers University of Technology
Computer labs · 1st year MSc Nanotechnology · 2 h/week

2018–2021 — **Physical chemistry**
Chalmers University of Technology
Tutorials and experimental labs · 2nd year BSc Biotechnology · 12 h/week

2018–2021 — **Theoretical chemistry**
Chalmers University of Technology
Computer labs · 3rd year BSc Chemical engineering · 4 h/week

2017–2018 — **Chemistry and biochemistry**
Chalmers University of Technology
Experimental labs · 1st year BSc Chemical engineering · 8 h/week

2014 — **Calculus**
Chalmers University of Technology
Exercise sessions · 1st year BSc Chemical engineering · 1 h/week

PEDAGOGICAL TRAINING

2019 — **Teaching, learning and evaluation**
Chalmers University of Technology
3 ECTS

SUPERVISION OF STUDENTS

Since 2024 — Supervisor of MSc student — Aalto University

Since 2024 — Advisor of PhD student — Aalto University

Since 2022 — Co-supervisor of PhD student — University of Helsinki

11/2024 – 5/2024 — Supervisor of BSc student — Aalto University

5/2021 – 9/2021 — Co-supervisor of 2 visiting and 3 BSc students — Chalmers University of Technology

1/2021 – 6/2021 — Co-supervisor of 6 BSc students — Chalmers University of Technology

6/2020 – 8/2020 — Supervisor of 2 BSc students — Chalmers University of Technology

1/2020 – 6/2020 — Supervisor of 6 BSc students — Chalmers University of Technology

4/2019 – 7/2019 — Supervisor of visiting BSc students — Chalmers University of Technology

4/2018 – 6/2018 — Supervisor of one BSc student — Chalmers University of Technology

SKILLS AND COMPETENCES

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

LANGUAGES

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

AWARDS AND HONOURS

2025 — **Marie Skłodowska-Curie postdoctoral fellowship**
202,000 EUR

2024–2025 — **LUMI extreme scale access resource allocation**

2018–2021 — **Travel grants**
Nils Philblad Foundation (2021) · Karl and Annie Leon's Foundation (2018–2019)

ACADEMIC SERVICE

2026 — Thesis reviewer and opponent — Universitat Autònoma de Barcelona (UAB), Barcelona, Spain

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

2023 — Organizer of workshop hands-on session — Shaking Up Tech, Workshop for underrepresented groups in STEM, Aalto University, Finland

2023 — Session chair and organizer — ESTML, Levi, Finland

2022 — Session chair — AbSciCon, USA

PEER-REVIEWED PUBLICATIONS

15 peer-reviewed articles, 6 first author. Total citations: 141, h-index: 5, i10-index: 5 — Google Scholar, updated 2 April 2026

15. Cappelletti, M., **Sandström, H.**, & Rahm, M. *ACS Central Science*, 12, 111–121 (2026). DOI: 10.1021/acscentsci.5c01497.
14. Lind, L., **Sandström, H.**, & Rinke, P. *The Journal of Chemical Physics*, 164 (2026). DOI: 10.1063/5.0308548.
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. Brean, J., Bortolussi, F., Rowell, A., Beddows, D. C. S., Weinhold, K., Mettke, P., Merkel, M., Kumar, A., Barua, S., Iyer, S., Karppinen, A., **Sandström, H.**, Rinke, P., et al. *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. Izquierdo-Ruiz, F., Cable, M. L., Hodyss, R., Vu, T. H., **Sandström, H.**, Lobato, A., & Rahm, M. *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. Valiev, R. R., Nasibullin, R. T., **Sandström, H.**, Rinke, P., Puolamäki, K., & Kurten, T. *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.**, Partovi, F., Mikkilä, J., Rinke, P., & Rissanen, M. *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.**, Hofmann, A. E., Hodyss, R., Rensmo, L., van der Meulen, M., Rahm, M., Cable, M. L., & Lunine, J. I. *Astrobiology*, 25, 367–389 (2025). DOI: 10.1089/ast.2024.0125. *[Performed geometry optimizations, conformer search and student supervision.]*
7. **Sandström, H.**, & Rinke, P. *Geoscientific Model Development*, 18, 2701–2724 (2025). DOI: 10.5194/gmd-18-2701-2025.
6. **Sandström, H.**, Rissanen, M., Rousu, J., & Rinke, P. *Advanced Science*, 11, 2306235 (2024). DOI: 10.1002/advs.202306235.
5. **Sandström, H.**, Izquierdo-Ruiz, F., Cappelletti, M., Dogan, R., Sharma, S., Bailey, C., & Rahm, M. *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., Sriram, K. K., Müller, V., Öz, R., **Sandström, H.**, Åhrén, C., Westerlund, F., & Karami, N. *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.]*

TALKS

INVITED SEMINARS AND KEYNOTES

2026	**Data-driven compound identification with atmospheric mass spectrometry** *Network on Mathematical Data Science for Materials Science, Workshop on the Interface of Mathematics and Machine Learning for Applications in Materials Science — University of Glasgow, UK*
2025	**CLOUDMAP – Advanced identification of atmospheric compounds** *Atmospheric day, Sweden — **Keynote***
2025	**Machine learning for atmospheric mass spectrometry** *Nordic Workshop on AI for Climate Change, Sweden*
2024	**AI in Chemistry: Solving experimental challenges with artificial intelligence** *FysKemDagarna (Physics and Chemistry Days), Sweden*

CONTRIBUTED TALKS

2026	**Towards atmospheric compound identification using simulated electron ionization mass spectra** *Chemical Compounds Space Conference (CCSC 2026), Munich, Germany*
2023	**Characterizing Atmospheric Molecules for Machine Learning** *International Aerosol Modeling Algorithms Conference, USA*
2023	**Characterizing Atmospheric Molecules for Machine Learning** *European Aerosol Conference, Spain*
2023	**Characterizing atmospheric molecules for machine learning** *Physics Days, Finland*
2022	**Untangling hydrogen cyanide polymerization using quantum chemistry** *AbSciCon, USA*