Rohit Goswami

https://rgoswami.me

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EDUCATION

UNIVERSITY OF ICELAND
Ph.D. Physical Sciences
2019 -- 2025 | Reykjavík, Iceland
Bayesian ML for magnetic interactions

HBTU KANPUR
B.Tech. in Chemical Engineering
2018 | Kanpur, India
First Division

DPS KALYANPUR
Intermediate (AISSCE)
May 2013 | Kanpur, India
CBSE, 87.2%

High School (AISSE)
May 2011 | Kanpur, India
CBSE, CGPA 9.8

MEMBERSHIPS

CURRENT
APS, 2015, Early Career
IEEE, 2015, Early Career
IOP, 2015, Member (MInstP)
AIChE, 2015, Young Professional
ACM, 2019, Professional
RSC, 2022, Member (MRSC)
BCS, 2022, Professional (MBCS)

SKILLS

SIMULATION
LAMMPS • ORCA • AiiDA • OVITO • ESPResSoMD • GROMACS • VMD • CMake

CREATED
d-SEAMS • wailord • fastMatMR • zenYoda • docuYoda

PROGRAMMING
C++ • Python • R • Fortran • Rust • Julia • Shell • LaTeX • Nix • JS • CUDA

EXPERIENCE

LAB COSMO, EPFL | Systems Specialist (Postdoc)
2025 -- Present | Lausanne, Switzerland

Working with Prof. Michele Ceriotti and Dr. Guillaume Fraux on the `metatensor` ecosystem for interoperable atomistic machine learning, including GROMACS integration and DLPack support.

QUEEN'S UNIVERSITY | Visiting Researcher
2025 | Kingston, Canada
Scaling off-lattice kinetic monte carlo to over a million atoms with Prof. Laurent Béland.

UNIVERSITY OF ICELAND | Doctoral Researcher
2019 -- 2024 | Reykjavík, Iceland
Rannís Doctoral Grant PI: Bayesian ML for saddle point searches on potential energy surfaces. Supervised by Prof. Hannes Jónsson.

QUANSIGHT LABS | Software Engineer II
2021 -- 2025 | Remote
Maintained `f2py` (NumPy) and foundational FOSS scientific codebases.

IIT KANPUR | Senior Project Associate / Project Associate
2018 -- 2020 | Kanpur, India
- Computational nanoscience: ice structure analysis (CHILL+), GPU-accelerated MD tools
- Femtolab: quantum information and computation with ultrafast lasers

PUBLICATIONS

SELECTED | JOSS Editor (2024--present)

[1] Filippo Bigi, Joseph W. Abbott, Philip Loche, Arslan Mazitov, Davide Tisi, Marcel F. Langer, Alexander Goscinski, Paolo Pegolo, et al. *Metatensor and Metatomic: Foundational Libraries for Interoperable Atomistic Machine Learning*. Aug. 2025. doi: `10.48550/arXiv.2508.15704`. arXiv: `2508.15704 [physics]`. (Visited on 09/04/2025).

[2] Rohit Goswami, Maxim Masterov, Satish Kamath, Alejandro Pena-Torres, and Hannes Jónsson. "Efficient Implementation of Gaussian Process Regression Accelerated Saddle Point Searches with Application to Molecular Reactions". In: *Journal of Chemical Theory and Computation* (July 2025). doi: `10.1021/acs.jctc.5c00866`. arXiv: `2505.12519`.

[3] Rohit Goswami, Amrita Goswami, and Jayant Kumar Singh. "d-SEAMS: Deferred Structural Elucidation Analysis for Molecular Simulations". In: *Journal of Chemical Information and Modeling* (Mar. 2020). issn: 1549-9596. doi: `10.1021/acs.jcim.0c00031`. arXiv: `1909.09830`.

SELECTED SERVICE & AWARDS

- **JOSS Editor** (2024–present); **NumFOCUS GSoC Admin** (2024–present)
- **IEEE P3173 Vice Chair**; **Nordic-RSE** Board, founding Secretary
- **COST Action Co-Proposer** (575k EUR, 2025–2029); **Rannís Doctoral Grant** (6650k ISK)
- **Reviewer**: Nature Comms, PRL, PRA, PRE, JOSS (80+), PLOS ONE, IOP, PeerJ
- **Teaching**: Stanford CS106A, The Carpentries, University of Iceland