Last updated on January 28, 2022

Amrita Goswami

House No. 646, 35th Lane
IIT Kanpur, 208016
+91 8874170409
amritag@iitk.ac.in
amritagos
https://github.com/amritagos/

"Avoid the temptation to work so hard that there is no time left for serious thinking."
– Francis Crick

Personal Data

Name Amrita Goswami
Date Of Birth 16.08.1991

Education

2016–present **MS-Ph.D. Chemical Engineering**, *Indian Institute of Technology*, Kanpur, *India*.
8.75 CGPA (Advisor: Prof. Jayant K. Singh; Co-Advisor: Prof. Indranil Saha Dalal)

2012–2016 **B.Tech. Chemical Engineering**, *Harcourt Butler Technical University*, Kanpur, *India*.
72.36% First Division (Project: Sulphur Acid Production optimization via the Chamber Process)

2008–2010 **Intermediate (AISSCE)**, *The Jain International School*, Kanpur, *India*.
85% Central Board of Secondary Education (CBSE)

2006–2008 **High School (AISSE)**, *Delhi Public School Kalyanpur*, Kanpur, *India*.
93% Central Board of Secondary Education (CBSE)

Technical Skills

Programming Languages

Experienced C++(11,17), FORTRAN 90, Tcl, R, C99, Shell (zsh,bash)

Familiar Julia, Python(2.7 and 3.6), FORTRAN 2008

Simulation Packages

Experienced LAMMPS (Large-scale Atomic /Molecular Massively Parallel Simulator) for Nucleation, Nanoparticles and wetting, VMD (Visual Molecular Dynamics), Ovito

Familiar ESPResSo (Extensible Simulation Package for Research on Soft matter), OpenFOAM, GROMACS (GROningen MAchine for Chemical Simulations), AMBER

Tools

Experienced gnuplot,XǝLaTeX, sed, awk, Git (version control), tmux, ssh, Sublime Text Editor 3, Vim, gadfly, i3 (tiling window manager), mosh, babun, MATLAB (matrix laboratory), markdown, Photoshop

Familiar moltemplate, Office-Suites (MS, OpenOffice, LibreOffice)

Research Topics

Experienced Ice nucleation, NEMD, Molecular Dynamics simulations, Phase transitions, Classical Nucleation Theory, Structure elucidation, High performance open source software, Scientific Software Development

Interested Molecular modeling, Free energy analysis, Optimal time-stepping methods, Accelerated simulations, HPC Algorithms

Accolades & Affiliations

Awards

November 2019 **RSC Physical Chemistry Chemical Physics Poster Prize**, *DAE Computational Chemistry Symposium, BARC, India*.

February 2020 **Springer Poster Award**, *Molecular Simulations of Complex Fluids and Interfaces, IIT Kanpur*.

November 2019 **Hot PCCP Article**, Article selected as a '2019 HOT PCCP Article', and as an inside front cover.

Memberships

2014–present **AIChE (American Institute Of Chemical Engineers)**, *Student Member*.

2018–present **OSA (Optical Society of America)**, *Student Member*.

Experience

Teaching

2016–present **Teaching Assistant**, *Indian Institute of Technology, Kanpur*, I have been a teaching assistant for the undergraduate courses 'Chemical Engineering Thermodynamics' and 'ESO-201, Thermodynamics'.

July–August 2020 **Water, Chemicals and more with Computers for Chemistry (WC3m)**, *Wave Learning Festival*, 15 hour long summer course for high school students and undergraduates on the basics of computational chemistry.

Winter 2020–present **NPTEL Chemical Engineering Thermodynamics**, *Indian Institute of Technology Kanpur*, I am a teaching assistant for an online national course organized by Indian Institutes of Technology and Indian Institute of Science.

Reviews

2019–present **Journal of Open Source Software**, *Reviewer*.

2019–present **PeerJ-Computer Science**, *Reviewer*.

Grants Awarded

2020–2023 **Icelandic Research Fund**, *Rannís*, 11.550 thousand ISK, Post Doctoral Fellowship.
Title: Modeling of transport and crystal nucleation in aqueous ionic solutions under shear.

Publications

Journals

[1] Amrita Goswami and Jayant K. Singh. "A general topological network criterion for exploring the structure of icy nanoribbons and monolayers." In: *Phys. Chem. Chem. Phys.* 22 (7 2020), pp. 3800–3808. DOI: 10.1039/C9CP04902A.

[2] 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.

[3] Amrita Goswami and Jayant K. Singh. "Exploring the Anomalous Phase Behavior of High-Pressure Ices in Diamond Confinement." In: *The Journal of Physical Chemistry C* 124.9 (2020), pp. 5460–5468. DOI: 10.1021/acs.jpcc.9b11531.

[4] Amrita Goswami, Indranil Saha Dalal, and Jayant K. Singh. "Seeding method for ice nucleation under shear." In: *The Journal of Chemical Physics* 153.9 (2020), p. 094502. DOI: 10.1063/5.0021206.

[5] Amrita Goswami and Jayant K. Singh. "A Hybrid Topological and Shape-Matching Approach for Structure Analysis." In: *The Journal of Chemical Physics* 154.15 (Apr. 2021), p. 154502. DOI: 10.1063/5.0046419.

[6] Amrita Goswami, Indranil Saha Dalal, and Jayant K. Singh. "Universal Nucleation Behavior of Sheared Systems." In: *Physical Review Letters* 126.19 (May 2021), p. 195702. DOI: 10.1103/physrevlett.126.195702.

[7] Amrita Goswami and Jayant K. Singh. "Homogeneous Nucleation of Sheared Liquids: Advances and Insights from Simulations and Theory." In: *Physical Chemistry Chemical Physics* 23.29 (July 28, 2021), pp. 15402–15419. ISSN: 1463-9084. DOI: 10.1039/D1CP02617H.

[8] Suraj K, Amrita Goswami, and Jayant K. Singh. "Salt-Water System under Diamond Confinement." In: *The Journal of Physical Chemistry C* 125.40 (Oct. 14, 2021), pp. 22283–22294. ISSN: 1932-7447. DOI: 10.1021/acs.jpcc.1c06410.

Conference Proceedings

[1] Rohit Goswami, Amrita Goswami, and Debabrata Goswami. "Space Filling Curves: Heuristics For Semi Classical Lasing Computations." In: *2019 URSI Asia-Pacific Radio Science Conference (AP-RASC)*. Mar. 2019, pp. 1–4. DOI: 10.23919/URSIAP-RASC.2019.8738612.

[2] Amrita Goswami and Jayant K. Singh. "General topological network criteria and implementation for monolayers and ice nanotubes." In: *ACS Spring 2020 National Meeting & Expo*. Mar. 2020. DOI: 10.1021/scimeetings.0c00176.

Conferences, Symposia & Workshops

Posters

7-9 November 2019 **DAE Computational Chemistry Symposium, BARC**, *Mumbai*, A Family of General Topological Network Criteria for Confined Ice Structure Determination.

21-23 February 2020 **Molecular Simulations of Complex Fluids and Interfaces**, *IIT Kanpur*, Formulation and Implementation of General Topological Network Criteria for Exploring the Structures of Confined Ice.

Attended

December 2017 **RARE Symposium**, *Agra*.

July 2019 **Rare Events Summer School**, *Indian Institute of Science, Bangalore*, A short course consisting of lectures and hands-on sessions by experts in the field, organized by Prof. Baron Peters.

21 September 2019 **OpenACC GPU Bootcamp**, *Indian Institute of Technology, Kanpur*, Day long programming session and discussion covering the acceleration of Institute in-house code by a Senior NVIDIA Solution Architect.

Relevant Coursework

2017 Spring **Molecular Modelling In Chemistry**, *CHM695*, Instructor: Prof. Nisanth Nair, **Grade: A***.

2017 Fall **Intermolecular and Surface Forces**, *CHE625A*, Instructor: Prof. Animangsu Ghatak, **Grade: A.**

2016 Spring **Introduction to Molecular Simulations**, *CHE622A*, Instructor: Prof. Martin Horsch, **Grade: B.**

Miscellaneous

Internships

Summer 2015 **Prof. Krishanu Ray**, *Tata Institute for Fundamental Research, Mumbai*, VSRP Fellow.
Worked on micro-channel flow modeling with OpenFOAM and produced a working prototype with the machine shop of TIFR. Also attended lectures over eight weeks as a part of the program.
Project Report: Design of a flow-cell for TIRFM imagining of Kinesin-2

Winter 2014 **Prof. Animangsu Ghatak**, *Indian Institute of Technology Kanpur*, Research Intern.
Worked on the imaging of programmable micro-lenses of oil on a PDMS substrate.

Volunteer Work

2017–2018 **ChemE Research Scholar Day**, *Indian Institute of Technology, Kanpur*, Anchor.
Managed and spearheaded the festivities of the research oriented student presentations and posters.

February 2019 **FunMolSim Workshop**, *Indian Institute of Technology, Kanpur*, Organizer, Helped organize, designed and taught tutorials at a pedagogical workshop for molecular dynamics.

2017–2020 **Animal Welfare Group**, *Indian Institute of Technology, Kanpur*, Member.
Rescued and fostered stray and injured animals.