Amrita Goswami

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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)

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)

Experience

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.

2012–2016 **The Curiosity Magazine**, *Harcourt Butler Technical University, Kanpur*, Editor-in-Chief.
Managed a diverse team of student content writers and rose from the ranks of writer in first year to the Editor-in-Chief by the third year.

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, XeLaTeX, 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 Interests

Experienced	Nucleation, NEMD, Molecular Dynamics simulations, Phase transitions, Thermodynamics, Statistical Mechanics, Structure elucidation, High performance open source software
Interested	Molecular modeling, Free energy analysis, Optimal time-stepping methods, Accelerated simulations, Optics

Affiliations & Accolades

Memberships

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

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

Awards

March 2014 **Resonance Short Story Competition**, *Harcourt Butler Technological Institute, Kanpur*, First Prize.

Publications

Journals

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.

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. eprint: https://doi.org/10.1021/acs.jpcc.9b11531. URL: https://doi.org/10.1021/acs.jpcc.9b11531.

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. URL: http://dx.doi.org/10.1039/C9CP04902A.

Conference Proceedings

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.

Preprints

Amrita Goswami, Indranil Saha Dalal, and Jayant K. Singh. *Seeding Method For Ice Nucleation Under Shear*. 2020. arXiv: 2006.14919.

Conference Records

Attended

DECEMBER 2017 **RARE Symposium**, *Agra*.

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.**