Sachin MB Gautham

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⦿ GauthamMBS   🌐 https://sites.google.com/smail.iitm.ac.in/prg

Education

2020 – Ongoing	🔖 **Ph.D.in Chemical Engineering** Indian Institute of Technology Madras (IITM). CGPA: 7.81
2017 – 2019	🔖 **M.E in Chemical Engineering** Birla Institute of Technology and Science (BITS) Pilani, K.K. Birla Goa Campus, India. CGPA: *8.49*
2013 – 2017	🔖 **B.Tech in Chemical Engineering** National Institute of Technology Karnataka Surathkal (NITK), India. CGPA: *7.56*

Research Experience

Jan 2020 – Ongoing	🔖 **Ph.D.in Chemical Engineering** Indian Institute of Technology Madras (IITM). Developed generic kremer grest based coarse-grained model of the grafted nanoparticle. Studied phase behavior of the GNPs. Developed coarse-grained model of non-spherical nanoparticles and evaluated their shear viscosity using molecular dynamics simulations. Studied anisotropic self-assembly of nanoparticles in a polymer matrix using molecular dynamics simulations. Predicted the effective potential of mean force between two polymer grafted nanoparticles using machine learning based MD simulations.
2017 – 2019	🔖 **M.E in Chemical Engineering** Birla Institute of Technology and Science (BITS) Pilani, K.K. Birla Goa Campus, India. CGPA: *8.49*
2013 – 2017	🔖 **B.Tech in Chemical Engineering** National Institute of Technology Karnataka Surathkal (NITK), India. CGPA: *7.56*

Academic Training

Ph.D.

2019-present	🔖 **Molecular Dynamics:** Proficient in running MD simulations using advanced techniques such as **Coarse-grained MD Simulations, Polymer Nanocomposite based Simulation, Machine Learning based Potentials (MLP).**
	🔖 **Visualization:** Proficient in running visualization tools such as **Ovito, and VMD.**
	🔖 **Computational Languages:** Efficient in Languages such as **Python, FORTRAN, MATLAB, and LINUX.**

Postgraduate

| 2017-2019 | 🔖 **Analytical Tools:** UV-Vis Spectrophotometer, Doctor-Blade, Ubbelohde Viscometer and Orbital Ultrasonicator. |

Teaching Proficiency

Undergraduate and Postgraduate

Theory and Tutorial   ◼ **Teaching Assistant** Heat Transfer, Mass Transfer, Chemical Engineering Thermodynamics, Advanced Process Control, Membrane Technology, Molecular Data Science and Informatics, Machine Learning in Reaction Engineering.

Lab   ◼ **Teaching Assistant** Computational Programming and Process Simulation, Computational Techniques.

Mentoring

Jun 2022   ◼ **M.Tech**. Self Assembly of Nanoparticles in a Polymer Matrix Using MD Simulation (Mr.Abishek Seth).

◼ **M.Tech**. Phase Behavior of Non-spherical Nanoparticles in a Polymer Matrix Using MD Simulation (Ms.Sayani Karmakar)

Research Publications

Journal Articles

1   K. R. Venkatachalam, **S.M.B Gautham**, and J. N. Nambi Krishnan, "Desalination characteristics of new blend membranes based on sulfonated polybenzimidazole and sulfonated poly(arylene ether sulfone)," *Polymer Bulletin*, vol. 80, no. 7, 2023. 🔗 DOI: `10.1007/s00289-022-04428-3`.

2   A. A. Bale, **S.M.B Gautham**, and T. K. Patra, "Sequence-defined Pareto frontier of a copolymer structure," *Journal of Polymer Science*, vol. 60, no. 14, pp. 2100–2113, 2022. 🔗 DOI: `10.1002/pol.20220088`.

3   **S.M.B Gautham** and T. K. Patra, "Deep learning potential of mean force between polymer grafted nanoparticles," *Soft Matter*, vol. 18, no. 41, pp. 7909–7916, 2022, The Royal Society of Chemistry. 🔗 DOI: `10.1039/D2SM00945E`.

4   K. R. Venkatachalam, **S.M.B Gautham**, A. Anegondi Nateri, and J. Nambi Krishnan, "Nano-enhanced sulfonated poly(arylene ether sulfone) composite membranes and their characterization," *High Performance Polymers*, vol. 34, no. 10, pp. 1193–1203, 2022, SAGE Publications. 🔗 DOI: `10.1177/09540083221112306`.

Conference Proceedings

1   **S.M.B Gautham** and T. Patra, "Predicting Polymer Grafted Nanoparticles Assembly using Deep Learning," APS March Meeting Abstracts, 2023, N00.002. 🔗 URL: `https://ui.adsabs.harvard.edu/abs/2023APS..MARN00002G`.

Skills

Languages   ◼ Strong reading, writing, and speaking competencies in English, Tamil (Mother Tongue), Kannada, and Hindi.

Tools   ◼ Python, MATLAB, LaTeX, FORTRAN, LAMMPS, and Microsoft Office

Misc.   ◼ Academic research, teaching, training, consultation, LaTeX typesetting, and publishing.

Miscellaneous Experience

Awards and Achievements

2023   **Chemplus 2023**, Received First Place in Paper Presentation Titled "Predicting Polymer Grafted Nanoparticles Assembly using Deep Learning ".

Argonne National Lab ,Received 100,000 node-hours of computing time on HPC by drafting a successful research proposal.

Partial Travel Funding, Received International Travel Assistance from the Institute To Attend a Conference.

American Physical Society, Attended The APS March Meeting to Present my Poster in Las Vegas, Nevada.

EESTER23, Conducted Hands-on Workshop on Machine Learning Potentials using AeNET and LAMMPS package in SRM College of Engineering, KTR Campus, Chennai.

2018   **InDA 2018**, Received First Place in Poster Presentation Titled "Sulfonated-PBI Based Blend Membranes For Desalination" in NIT Trichy.

References

Available on Request