Sachin MB Gautham Curriculum Vitae

#E003, Department of Physical Sciences, IISc Bengaluru 560012 | +91 9482140436 | sachingthm7@gmail.com

Summary

Interdisciplinary researcher with a Ph.D. in Chemical Engineering from IIT Madras and current postdoctoral experience at IISc Bengaluru. Expert in statistical thermodynamics and soft matter physics, with a specialized focus on multi-scale molecular modeling and machine learning. Proven expertise in utilizing exascale computing to solve complex challenges in polymer science and nanocomposite systems. I seek to establish an independent, interdisciplinary research laboratory that integrates molecular theory, high-fidelity simulations, and AI-driven optimization to accelerate the design of functional nanomaterials. Committed to academic excellence through high-impact research, securing external funding, and fostering a rigorous pedagogical environment.

Education

- **PhD**, Chemical Engineering, Indian Institute of Technology (IIT) Madras, Feb 2026
- **M.E**, Chemical, Birla Institute of Technology and Science (BITS) Pilani, May 2019
- **B. Tech**, Chemical, National Institute of Technology (NIT) Karnataka, Surathkal, July 2004

Awards & Fellowships

- Won **First Prize for Best Poster** Presentation at PCCP-SPHERE 2025 (IISc) for the work titled "Thickening of Liquids Using Copolymer Grafted Nanoparticles."
- Awarded the **International Travel Scheme** (ITS) Grant by the DST, Govt. of India, to present doctoral research at the 12th International Liquid Matter Conference (2024) at the Max Planck Institute for Polymer Research, Mainz, Germany.
- Secured a high-performance computing allocation of **1,000,000 core-hours** (CNM 83298) at the **Argonne National Laboratory (Carbon Cluster), USA**, for large-scale simulations of nanomaterial assemblies (2023).
- Recipient of a competitive **Institute Travel Grant** from IIT Madras to present Ph.D. research at a specialized materials symposium in the USA (2023).
- Awarded **First Prize for Best Paper Presentation** at ChemPlus 2023 for developing a deep learning framework titled "Predicting Polymer Grafted Nanoparticles Assembly using Deep Learning."
- Completed Professional Industrial Training at JSW Steel (Hospet), gaining hands-on exposure to Syn-gas production technologies and smelter furnace operations(2014).

Research Experience

January 2026 – Present: **Research Associate – I**, Indian Institute of Science, Bengaluru, India

Advanced Atmospheric Water Harvesting (AWH) using Metal-Organic Frameworks (MOFs) and Covalent Organic Frameworks (COFs).

- Served as a lead computational researcher on a high-impact industrial-scale water harvesting project centered on CALF-20 and specialized COF architectures.
- Executed extensive Grand Canonical Monte Carlo (GCMC) simulations to rigorously evaluate multi-cycle water adsorption isotherms and hydrolytic stability of candidate MOF/COF structures.
- Developing a Machine Learning Potentials (MLPs) to overcome the computational bottleneck of traditional force-field methods, accelerating water-uptake prediction speeds by orders of magnitude without sacrificing atomistic accuracy.
- Analyzed complex simulation datasets to derive structure-property relationships, directly informing the optimization of water capture efficiency and regeneration energy for industrial-scale deployment.
- Bridged the gap between fundamental molecular theory and engineering application through high-fidelity performance modeling and active participation in cross-functional technical discussions with experimental partners.

July 2025 – December 2025: **Postdoctoral Fellow**, Accenture – IISc Bengaluru

IISc-Accenture Collaborative Initiative on Predictive Analytics for Polymeric Coatings.

- Spearheaded a collaborative research effort between IISc and Accenture to develop a predictive machine learning framework for the next generation of industrial paint formulations.
- Developed high-fidelity molecular models for complex ternary systems involving Poly(methyl methacrylate) (PMMA), Polystyrene (PS), and Titanium Dioxide (TiO_2) nanoparticles to investigate interfacial physics and dispersion stability.
- Architected a data-driven model to map molecular-level descriptors (polymer architecture, grafting density, and nanoparticle loading) to macroscopic rheological and mechanical properties critical to the paint industry.
- Successfully utilized the framework to predict key performance metrics such as viscosity profiles, pigment dispersion quality, and film-forming characteristics, significantly reducing the experimental trial-and-error cycle.
- Leading the translation of fundamental soft matter physics into actionable insights for industrial scale-up; ongoing optimization of NPs is yielding highly promising preliminary results in enhancing coating durability and opacity.
- Overseeing technical deliverables and regular progress briefings for industrial partners, computational frameworks have received positive stakeholder validation for their high degree of alignment with commercial formulation benchmarks and real-world performance requirements.

Aug, 2008 – July, 2012: **Institute Research Fellow**, IIT Madras, Chennai, India

Deep Learning Frameworks for Potential of Mean Force (PMF) in Polymer-Grafted Nanoparticles (PGNs)

- Developed a novel deep learning architecture to map the PMF between PGNs, enabling the rapid exploration of high-dimensional interaction landscapes that are traditionally computationally exhaustive.
- Engineered a robust data-generation pipeline that integrates advanced MD sampling techniques with neural networks to produce high-fidelity thermodynamic training datasets.
- Optimized deep learning models to predict interparticle interactions across a wide design space, including variations in grafting density, chain length, and solvent quality, ensuring the framework's versatility for different systems.
- Developed phase diagram of a polymer nanocomposite based on molecular dynamics simulations.
- Disseminated findings through high-impact peer-reviewed publications and presentations at international forums, contributing a scalable computational paradigm to the field of soft matter physics.

Nanotetrapods Promote Polymer Flow Through Confinement-Induced Packing Frustration

- Investigated anisotropic self-assembly of nanoparticles in a polymer matrix using molecular dynamics simulations.
- Developed a computational framework to model various nanoparticle geometries in nanocomposites.
- Identified the correlation between nanoparticle shapes and the rheology of nanocomposites and elucidated the molecular mechanism behind shape-dependent viscosity.
- Created a coarse-grained model for non-spherical nanoparticles and predicted their self-assembly behavior using molecular dynamics simulations.
- Collaborated with Prof. Mithun Chowdhary's lab (IITB) to validate the coarse-grained model with experimental data.

Sequence-Defined Pareto Frontier of a Copolymer Structure

- Developed a computational framework for designing copolymer sequences using genetic algorithms and molecular dynamics simulations.
- Analyzed structure-property correlations, such as radius of gyration, from a large collection of copolymer sequences.

Aug, 2007 – May, 2008: **Researcher**, BITS Pilani, Goa, India

Nano-Enhanced Sulfonated Poly (Arylene Ether Sulfone) Composite Membranes and Their Characterization.

- Designed and synthesized sPBI-SPAES with TiO_2 nanocomposite membranes for enhanced desalination properties.
- Casted and characterized reverse osmosis membranes incorporating TiO_2 nanocomposites.
- Focused on improving desalination efficiency through the integration of nanocomposites in membrane structure.
- Conducted in-house synthesis of reverse osmosis membranes to optimize material properties.
- Enhanced mechanical properties of nanocomposite membranes compared to pristine membranes.
- Investigated the performance of TiO_2 nanocomposite membranes in reverse osmosis processes.
- Contributed significantly to publishing peer-reviewed journal articles based on the research.

Independent Research Projects

1. Title: Understanding Switching Dynamics of Tantalum Oxide and Titanium Oxide based Memristive Device Grant No. CNM55595, Agency: ANL, Allocation: 500000 CPUS hours of *Carbon* supercomputer, 2017
2. Title: Computational Modeling and Simulation Studies of Polymer Directed Assemblies of Nanoparticles: The effects of depletion force and anisotropic interaction, Grant No. DMR160016, Agency: XSEDE, Allocation: 592,594.27 CPU hours of *Stempede* supercomputer, Texas Advanced Computing Center, 2023.
3. Title: Polymer directed self-assembly of polymer grafted nanoparticles, Grant No. CNM 83298, Agency: Arogonne National Lab (ANL), Allocation: 1000,000 CPU hours of *Carbon* supercomputer, Center for Nanoscale Materials, 2024.

Mentorship Activities

1. Mentored Mr. Abhishek for MS thesis on "Glass transition in ion-containing polymers," (2021-2022)
2. Co-advised Ms. Sayani Karmakar for MS thesis on "Molecular dynamics simulation of ion transport in polymers," (2022 - 2023).

Teaching Experiences

- Teaching assistant at IIT Madras from August 2021 to July, 2024. The topics include thermodynamics, unit operation lab, introduction to molecular simulations, statistical thermodynamics, and thermodynamics of fluid mixtures
- Prepared course material including computer codes, lectures, homework, and practice problems
- Led weekly laboratory and/or problem-solving and discussion sessions
- Supervised undergraduate and graduate students in final projects, and weekly homework

Management & Services

- Member of American Institute of Chemical Engineers (AIChE), American Physical Society (APS) and Society of Polymer Science, India (SPSI)
- Member of organizing committee, ChemPlus school-cum-symposium, IIT Madras, Chennai, India, (2022)

Journal Publications

1. **Gautham S M B**, Sarkar J, and Patra T K, Flow Promoting Tetrapods- Nanoparticle Architecture Dependent Viscosity Reduction In PS Based Polymer Nanocomposites, Nature Communications 16, 8550 (2025)
2. **Gautham S M B**, Prama, Patra T K, Mondal T, and Kaushal M, Thickening of Liquids Using Copolymer Grafted Nanoparticles, Soft Matter 10, 5509 (2025)
3. **Gautham S M B**, and Patra T K, Deep Learning Potential of Mean Force Between Polymer Grafted Nanoparticles, Soft Matter 18, 7909 (2022)
4. Bale A, **Gautham S M B**, and Patra T K, Sequence-Defined Pareto Frontier of a Copolymer Structure, Journal of Polymer Science 60, 2100 (2022)

5. Venkatachalam K R, **Gautham S M B**, and Krishnan J N, Nano-Enhanced Sulfonated Poly (Arylene Ether Sulfone) Composite Membranes and Their Characterization, High Performance Polymers 34, 1193 (2022)
6. Venkatachalam K R, **Gautham S M B**, and Krishnan J N, Blend membranes of sulphonated poly(arylene ether sulphone) and sulphonated polybenzimidazole and their characterization for desalination applications, Bulletin of Materials Science 47, 1 (2024)
7. Venkatachalam K R, **Gautham S M B**, and Krishnan J N, Desalination Characteristics of New Blend Membranes Based on Sulfonated Polybenzimidazole and Sulfonated Poly (Arylene Ether Sulfone), Polymer Bulletin 80, 7805-7824(2023)

Manuscripts Under Preparation and Review

1. **Gautham S M B**, Banerjee R, and Maiti P K, Optimizing water harvesting in TTBA COF: An advanced NVT+W approach (2026)
2. **Gautham S M B**, and Maiti P K, Tuning the Viscoelasticity of Paint Formulations using Copolymer Grafted Nanocomposites (2026)
3. **Gautham S M B**, Banerjee R, and Maiti P K, Molecular mechanisms of water adsorption in functionalized Covalent Organic Frameworks (2027)
4. **Gautham S M B**, and Patra T K, Machine learning guided design of multi-component copolymer nanocomposites for industrial coatings (2027)

Thesis

1. **PhD thesis**: Microstructure – rheology correlations in polymer nanocomposites, submitted to IIT Madras, 2026
2. **M. Tech. thesis**: The synthesis of polymer nanocomposite membranes for desalination, submitted to BITS Pilani, 2019
3. **B. Tech. thesis**: Preparation and characterization of immobilized bacteria in sodium alginate, submitted to the NITK Surathkal, 2017

Talks and Poster Presentation

1. **Gautham S M B**, and Patra T K, Thickening of Liquids Using Copolymer Grafted Nanoparticles, RSC Physical Chemistry Chemical Physics (PCCP) SPHERE, IISc Bengaluru, India, October 2025
2. **Gautham S M B**, and Patra T K, Effects of nanoparticle shape on the rheology of a polymer nanocomposites, Liquid Matter Conference (LMC), Mainz, Germany, September 22-27, 2024
3. **Gautham S M B**, and Patra T K, Non-linear Rheology of Polymer Grafted Nanoparticle Solutions, Complex Fluids (CompFlu), Chennai, India, December 2023
4. **Gautham S M B**, and Patra T K, Predicting Polymer Grafted Nanoparticles Assembly using Deep Learning, Sustainable Polymer Society of India (SPSI) MACRO, Guwahati, India, December 2023
5. **Gautham S M B**, and Patra T K, Predicting Polymer Grafted Nanoparticles Assembly using Deep Learning, CECAM MD60, Bengaluru, India, September 2023
6. **Gautham S M B**, and Patra T K, Predicting Polymer Grafted Nanoparticles Assembly using Deep Learning, ChemPlus, IIT Madras, Chennai, India, March 2023
7. **Gautham S M B**, and Patra T K, Predicting Polymer Grafted Nanoparticles Assembly using Deep Learning, American Physical Society (APS) March Meeting, Las Vegas, Nevada, USA, March 5-10, 2023
8. **Gautham S M B**, and Patra T K, Predicting GNPs Assembly using Deep Learning, Complex Fluids (CompFlu), Kolkata, India, December 19-21, 2022