Sobin Alosious

Department of Mechanical Engineering | Massachusetts Institute of Technology, MA
(574) 300-8707 | sobin@mit.edu

RESEARCH INTERESTS

Nanoscale Thermal Transport, Molecular Simulations, Material Discovery, Polymer Informatics,, Energy Storage Materials, Nanofluidics, 2D Materials, Machine Learning, Artificial Intelligence.

POSTDOCTORAL APPOINTMENTS

2026-present	Postdoctoral Associate, Department of Mechanical Engineering, Massachusetts Institute of Technology, MA.
2024-2026	Postdoctoral Research Associate, Aerospace and Mechanical Engineering Department, Lucy Family Institute for Data and Society, University of Notre Dame, IN.
2022-2024	Postdoctoral Research Associate, Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, Australia.
2022	Institute Postdoctoral Researcher, Department of Applied Mechanics and Biomedical Engineering, Indian Institute of Technology Madras, India.

EDUCATION

2022	Ph.D. Jointly from the Indian Institute of Technology Madras, India, and Swinburne University of Technology, Australia. Thesis: "Study of Kapitza Resistance in Nano-confined Fluids"
2016	M.Tech Thermal Science, Kerala University, India. Thesis: "Experimental and Numerical Study on Heat Transfer Enhancement of Flat-Tube Radiator Using Al_2O_3 and CuO Nanofluids".
2013	B.Tech. Mechanical Engineering, Mahatma Gandhi University, India.

PUBLICATIONS

2026 "ADEPT-PolyGraphMT: automated molecular simulation and multi-task multi-fidelity machine learning for polymer property generation and prediction" *Digital Discovery*, (2026).

2026 "Study of the Molecular Level Mechanism of Nanoscale Alternating Current Electro-hydro-dynamic Flow." *International Communications in Heat & Mass Transfer*, (2026).

2026 "A Transfer Learning Framework Integrating Molecular Dynamics and Group Contribution Methods for Predicting Polymer Specific Heat Capacity." *Polymer Chemistry,* (2026).

2025 "Dofulator: A Tool for Calculating Degrees of Freedom of Atoms in Molecules with Geometry Constraints." *Computer Physics Communications*, 110003 (2025).

2025 "Tunable Linear Weight Modulation via Ion Dynamics in Electrolyte-Gated Synaptic Transistors: Molecular Dynamics and Experimental Insights into Ion Concentration Effects." *Advanced Functional Materials* (2025), e17100.

2025 "Computation and Machine Learning for Materials: Past, Present, and Future Perspectives." *MRS Bulletin, Springer*, 1-13.

2025 "Machine Learning in Nanoscale Thermal Transport." *Annual Review of Heat Transfer, Begel House Inc,* 28 (2025).

2023 "Interfacial thermal transport and electrical performances of supercapacitors with graphene/carbon nanotube composite electrodes." *The Journal of Physical Chemistry C,* 128-5, 2190-2204.

2022 "Effects of Electrostatic Interactions on Kapitza Resistance in Hexagonal Boron Nitride-Water Interfaces." *Langmuir*, 38, 8783-8793.

2021 "Nanoconfinement Effects on the Kapitza Resistance at Water-CNT Interfaces." *Langmuir*, 37 (7), 2355-2361.

2020 "Kapitza resistance at water-graphene interfaces." *The Journal of Chemical Physics*, 152, 224703.

2019 "Prediction of Kapitza resistance at fluid-solid interfaces." *The Journal of Chemical Physics*, 151, 194502.

2018 "Investigations on convective heat transfer enhancement in circular tube radiator using Al_2O_3 and CuO nanofluids." *Journal of Thermal Science and Engineering Applications-ASME,* 10(5), 051012.

2017 "Experimental and numerical study on heat transfer enhancement of flat tube radiator using Al_2O_3 and CuO nanofluids." *Heat and Mass Transfer-Springer*, 53, 12, 3545-3563.

CONFERENCE PUBLICATIONS/PRESENTATIONS

2025 "Multi-Fidelity Machine Learning for Predicting Polymer Heat Capacity" *COSE Research Horizons Symposium,* University of Notre Dame, USA, November 2025.

2025 "Quest2DataAgent: Automating End-to-End Scientific Data Collection." *The 2025 Conference on Empirical Methods in Natural Language Processing (EMNLP 2025),* Pages 500-514, Suzhou, China, November 2025.

2025 "Multi-Fidelity Machine Learning for Predicting Polymer Heat Capacity" *10th Notre Dame-Purdue Symposium on Soft Matter & Polymers,* Purdue University, USA, November 2025.

2025 "Leveraging Transfer Learning and Molecular Simulations for Accelerated Polymer Property Prediction and Discovery." *The RISE AI Conference,* The University of Notre Dame, USA, October 2025.

2022 "The Effects of Electrostatic Interactions on Kapitza Resistance in Nano-Confined Water." *8th Statistical Mechanics of Soft Matter Meeting (SM2),* Monash University, Melbourne, Australia, July 2022.

2021 "Study of Kapitza Resistance at Fluid-Solid Interfaces in Planar and Cylindrical Nano-Confinement Systems." 21st Symposium on Thermophysical Properties, Joint ASME-AIChE Committee on Thermophysical Properties, University of Colorado, Boulder, USA, June 2021.

2021 "Study of interfacial thermal resistance in boron nitride nanotube (BNNT)-water interface." *26th National and 4th International ISHMT-ASTFE Heat and Mass Transfer Conference*, IIT Madras, Chennai, Tamil Nadu, India, December 2021.

2019 "Study of Kapitza resistance at planar solid-fluid interface in a Lennard-Jones system." *6th Statistical Mechanics of Soft Matter Meeting (SM2)*, University of Adelaide, Australia, December 2019.

2016 "Numerical Analysis on Cooling Performance of Automobile Radiator Using CuO-water Nanofluids." *National Conference on Technological Trends*, CET Trivandrum, India. August 18-20, 2016.

2016 "Numerical investigation of forced convective heat transfer in round tube radiators using aluminum oxide-water nanofluid." *National Conference on Technological Trends*, CET Trivandrum, India. August 18-20, 2016.

TEACHING EXPERIENCE

2025 Invited Instructor, Aerospace and Mechanical Engineering Department, University of Notre Dame – "Molecular Dynamics Simulations using LAMMPS."

2022 Invited Lecturer, Mechanical Engineering Department, College of Engineering Trivandrum, Kerala – "Introduction to Molecular Dynamics."

2019 Workshop Instructor, Department of Applied Mechanics and Biomedical Engineering, Indian Institute of Technology Madras, "Hands-on Workshop on LAMMPS Simulations."

2018 Teaching Assistant, Department of Applied Mechanics and Biomedical Engineering, Indian Institute of Technology Madras– "Fluid Mechanics."

2016 Assistant Professor, Mechanical Engineering Department, Holy Kings College of Engineering and Technology, Kerala – "Thermal Engineering.

AWARDS AND SCHOLARSHIPS

2022 Institute Predoc Award – Indian Institute of Technology Madras.
2019 Joint Ph.D. Fellowship Award, Indian Institute of Technology Madras & Swinburne University of Technology, Australia.
2014 GATE Scholarship – Ministry of Human Resource Development (MHRD), India.

CERTIFICATIONS AND WORKSHOPS

2025 Responsible Conduct of Research for Engineers, CITI Program.
2024 Supervised Machine Learning: Regression and Classification, DeepLearning.AI, Stanford University.
2017 Faculty Development Program – Viswajyothi College of Engineering and Technology, India.
2013 Orientation workshop for National Energy Auditing Competition by ECS, Government Engineering College, Thrissur, India.
2012 Robotic workshop by Robosapiens– Viswajyothi College of Engineering and Technology, India.
2011 AutoCAD Certified Associate, Autodesk.

PROFESSIONAL MEMBERSHIPS

2025-present Member, National Postdoctoral Association
2024-present Member, NDnano – Center for Nano Science and Technology, University of Notre Dame.
2024-present Member, Materials Research Society (MRS), University of Notre Dame.
2013 Volunteer Member, National Service Scheme (NSS), India.

PROFESSIONAL SERVICES

2025	Organizer, NeurIPS 2025 Open Polymer Challenge, NeurIPS + Kaggle Competition.
2025-present	Peer Reviewer, International Journal of Heat and Mass Transfer, Journal of Applied Physics, Physics of Fluids and Scientific Reports.
2018	Science Education Outreach program in rural villages in Tamil Nadu, India– IIT Madras.
2013	Rural Bio-Waste Management Installation – National Service Scheme (NSS), Kerala.

LANGUAGES

English (advanced reading, spoken, written).
Malayalam (advanced reading, spoken, written).

TECHNICAL SKILLS

Molecular Simulations: LAMMPS, VMD, Packmol, MDAnalysis, Pysimm, Psi4
Machine Learning: Python, PyTorch/TensorFlow, RDKit, Optuna, GNN, MLP
CFD & Engineering Tools: Ansys Fluent, AutoCAD, ICEM CFD.

REFERENCES

Gang Chen
Carl Richard Soderberg Professor of Power Engineering
Mechanical Engineering Department
Massachusetts Institute of Technology
(617) 253-0006
gchen2@mit.edu

Tengfei Luo
Professor
Aerospace and Mechanical Engineering Department,
University of Notre Dame, USA.
(574) 631-9683
tluo@nd.edu

Meng Jiang
Associate Professor
Computer Science and Engineering
University of Notre Dame, USA.
(574) 631-7454
mjiang2@nd.edu

Billy Todd
Professor
Department of Mathematics,
Swinburne University of Technology, Australia
+61 3 9214-8740
btodd@swin.edu.au

Debra Bernhardt
Professor
School of Chemistry and Molecular Biosciences,
The University of Queensland, Australia,
+61 7 334 63939
d.bernhardt@uq.edu.au

Sarith P Sathian
Professor
Department of Applied Mechanics and Biomedical Engineering,
Indian Institute of Technology Madras, India
+91 442 257 4062
sarith@iitm.ac.in