Curriculum Vitae

Samik Bose
Fixed-Term Assistant Professor
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Personal Statement: I am a **fixed-term assistant professor** in the Department of Computational Mathematics, Science and Engineering (CMSE) at Michigan State University. My current role has equal responsibilities towards **teaching** undergraduate courses and conducting **research** under the mentorship of **Prof. Alex Dickson,** my postdoctoral mentor. As a researcher, I aim to decipher long timescale molecular motions that play central roles in biophysics and chemistry by developing physics and machine leaning-based **reactive enhanced simulation** methods. Also, I am interested in exploring **kinetics** and **dynamics**-driven allosteric modulator design as an alternate paradigm of drug design. As an educator, I aim to practice evidence-based teaching methods with commitment towards a **diverse**, **equitable** and **inclusive** learning environment. I have been the lead instructor of a 400-level **Computational Medicine** course, where I **developed curriculum** covering topics from cancer genomics to AI-driven drug discovery to biomolecular simulation. I have been teaching multiple sections of a 300-level **Linear Algebra and Matrix Application** course. In future, the research outcome of my lab will augment drug discovery and enhance the understanding of fundamental chemistry and biology, promoting **collaboration** between in-vitro/in-vivo and in-silico approaches. I will create a healthy lab environment, promoting **diversity** and fostering an **equitable**, **inclusive** relation with **mentors, mentees** and **colleagues**.

WORK EXPERIENCES:

Fixed-Term Assistant Professor: August 2024 – current

Department of Computational Mathematics, Science and Engineering (CMSE)
Michigan State University, East Lansing, MI 48824, USA.

Postdoctoral Research Associate: January 2021 – August 2024

Department of Biochemistry and Molecular Biology **Supervisor: Dr. Alex Dickson**
Michigan State University, East Lansing, MI 48824

EDUCATION:

PhD in Chemistry September 2014 – September 2020

Indian Association for the Cultivation of Science, India **Supervisor: Dr. Debashree Ghosh**
Title of the thesis: “Polarization in Hybrid Quantum Mechanics/Molecular Mechanics Methods - Importance and Developments”.

Master of Science in Chemistry July 2012 – July 2014

University of Hyderabad, India CGPA: 8.0
Dissertation Topic: **Thermal fluctuation and dynamics in 2-D Frenkel-Kontorova chain.**
Relevant Courses: Stat. Mech. & Thermo., Electronic Structure, Spectroscopy, Chemical Kinetics.

Bachelor of Science in Chemistry July 2009 – July 2012

St. Xavier’s College, India Grade: A
Relevant Courses: Thermodynamics, Bioinorganic Chem, Quantum Mechanics, Chemical Kinetics.

FUTURE RESEARCH OBJECTIVES (IN BRIEF):

(1) Model **reactive rare events (slow processes) in complex biomolecular landscapes** by developing novel QM/MM- and ML/MM-driven reactive enhanced sampling molecular simulations.
(2) Map binding-to-reaction pathways, free energy and kinetics of **reversible covalent inhibitors in kinases** and understand the effect of slow environment motions in their **efficacy.**
(3) Utilize weighted ensemble based enhanced sampling strategy, combined with Markov state model to reveal the **biophysical basis of kinetics and dynamics driven allosteric modulator design for metallopeptidases and solute carrier transporter proteins.**

PUBLICATIONS:

- **S.Bose**, A. Aly, V. T. Karamyan, B. J. Orlando, A. Dickson, “Conformation Driven Enhancement of Neurolysin Activity in Presence of a Small Molecule Activator”. (Manuscript submitted to Biophysical Journal)
- H. E.L. ElZorkany, H. Kandil, S. Jayaraman, S. H. Esfahani, D. Patel, D. Dannecker, M. Maciag, A. Paul, K. Lowran, **S. Bose**, D. A. Ostrov, C. G. Wu, A. Dickson, T. J. Abbruscato, P. C. Trippier, B. J. Orlando, V. T. Karamyan, “Discovery of a pyridine-piperazine small molecule that enhances the activity of peptidase neurolysin”. (Manuscript submitted to The Journal of Pharmacology and Experimental Therapeutics)
- **S. Bose**, C. Kilinc, A. Dickson, “Markov State Models with Weighted Ensemble Simulation: How to Eliminate the Trajectory Merging Bias”, J. Chem. Theory Comput. **2025**, 21, 4, 1805–1816.
- **S. Bose**, S.D. Lotz, I. Deb, M.Schuck, K.S.S. Lee, A. Dickson, "How Robust is Ligand Binding Transition State", J. Am. Chem. Soc, **2023**, 145, 25318-25331.
- N. Donyapour, F.F. Niazi, N. Roussey, **S Bose**, A. Dickson, "Flexible Topology: A new method for dynamic drug design", J. Chem. Theory Comput., **2023**, 19, 5088-5098.
- **S. Bose**, S. Chakrabarty, D. Ghosh, “Support Vector Regression Based Monte Carlo Simulation of Flexible Water Clusters”, ACS Omega, **2020**, 5, 7065-7073.
- **S. Bose**, D. Dhawan, S. Nandi, R. R. Sarkar, D. Ghosh, “Machine Learning Prediction of Interaction Energies in Rigid Water Clusters”, Phys. Chem. Chem. Phys., **2018**, 20, 22987-22996.
- R. Chakraborty, **S. Bose**, D. Ghosh, “Effect of Solvation on the Ionization of Guanine Nucleotide: A Hybrid QM/EFP Study”, J. Comp. Chem., **2017**, 38, 2528-2537. (**Equal first authorship**)
- **S. Bose**, D. Ghosh, “An Interaction Energy Driven Biased Sampling Technique: A Faster Route to Ionization Spectra in Condensed Phase”, J. Comp. Chem., vol. **2017**, 38, 2248-2257.
- **S. Bose**, S. Chakrabarty, D. Ghosh, “Electrostatic Origin of the Red Solvatochromic Shift of DFHBDI in RNA Spinach”, J. Phys. Chem. B, **2017**, 121, 4790-4798.
- **S. Bose**, S. Chakrabarty, D. Ghosh, “Effect of Solvation on Electron Detachment and Excitation Energies of a Green Fluorescent Protein Chromophore Variant”, J. Phys. Chem. B, **2016**, 120, 4410-4420.

RESEARCH ACCOMPLISHMENTS:

- An enhanced sampling protocol (weighted ensemble) to **decipher inhibitor unbinding mechanism** and **kinetics** in pharmacologically relevant proteins: Providing a basis for **kinetics driven drug design** with insights from biomolecular rare events, **10^8 times slower** than simulation timescale.
- A method to integrate Markov state models with weighted ensemble enhanced MD simulations, two statistical mechanics driven powerful but conceptually different sampling methods to **achieve an order of magnitude gain** in **accuracy** in **predicting robust inhibitor binding kinetics**.
- Application of **machine learning algorithms** (i) in flexible topology simulations to **generate drug-like small molecule inhibitors** in protein binding pockets guided by free energy landscape, (ii) in building a **polarizable water model** for accurate description of interaction energies.
- Deciphering **binding site and mechanism of an allosteric modulator** in a clinically relevant protein neurolysin by computational modeling.
- Understanding the biophysics of small **molecular transport and signaling** through **transmembrane** proteins using enhanced sampling simulation tools.
- A biased sampling algorithm to construct **spectral features of chromophores in condensed phase** at **10^3 times lower** computational cost.
- Decoding the effect of RNA environment in the spectral shift of GFP chromophore variant using multiscale molecular modeling methods.

TEACHING/MENTORING EXPERIENCES:

Fixed-Term Assistant Professor:

(i) **Computational Medicine** (400-level): Lead instructor of 30 students (both undergrad and grad) Fall 2024 course. Solely developed a new curriculum for this course and implemented evidence-based teaching pedagogy (Flipped Classroom).

(ii) **Linear Algebra and Matrix Applications** (300-level): Instructor for a total of three sections (two in Fall 2025 and one in Spring 2025) of ~60 undergrads each. Co-developed rubrics of evaluation and course structure.

Postdoc:

(i) **Machine Learning for Molecular Dynamics** (900-level Biochemistry graduate course): Spring 2023, 2 self-developed modules (2 lab and 2 lectures), ~20 grad students.

(ii) **Mentoring** 4 undergraduate research assistants over a total of 6-8 semesters culminating **nominated and selected poster presentations, university credits.**

(iii) **Mentoring** graduate students in **DicksonLab** towards their PhD goals.

PhD:

(i) **Mentoring** ~6 undergraduate researchers/trainees culminating project presentations, posters and subjective outcomes.

(ii) **Mentoring** a C.V. Raman exchange fellow (a program to promote science and diversity) from Nigeria with the methods of quantum chemistry.

TECHNICAL SKILLS AND ASSETS:

- Part of **the software development and maintenance team** for DicksonLab software such as Wepy, CSNAnalysis, MLForce, MBC-MSM and Flexible topology.
- **10+ years of experience in scientific programming** (Python, R, Fortran, C) and necessary libraries.
- Proficient in both classical and quantum mechanical molecular modeling tools such as Openmm, Amber, Tinker, Charmm, Charmm-GUI, Gromacs, Q-chem, PySCF, Molpro, Gaussian.
- Expertise in employing **ML algorithms** such as diffusion models, CNNs, SVMs, clustering and dimension reduction methods using modules of scikit-learn, PyTorch, KernLab (in R).
- Expertise in **computer-aided drug discovery** with small molecule virtual screening and lead optimization softwares such as AutoDock, Schrodinger etc.
- Trained in **handling big data** in drug discovery related fields such as ChEMBL, GDB-13, QM-9 etc.
- Experienced in working with **experimental and computational collaborators** as part of a research team. Examples include cryo-EM specialists, spectroscopists, medicinal chemists etc.
- Equipped with teaching certifications such as CIRTL network offered **'An Introduction to Evidence-Based Undergraduate STEM Teaching'**.
- Ongoing training in **'Certification in College Teaching'** hosted by Michigan State University, Graduate Educator Advancement and Teaching Office.
- Strong communication (verbal and written) skills in English.
- Passionate about **collaboration**: Independently driving two collaborative projects with structural biologists and biochemists to resolve long-standing biomolecular mechanism questions.

ORAL AND POSTER PRESENTATIONS (SELECTED):

* Oral presentation: ***ACS Fall*** *(COMP Division),* August 2025, Washington DC.
* Poster presentation: ***Midwest Theoretical and Computational Chemistry Symposium***, May 2025, Wayne State University.
* Poster presentation: ***J1 Scholar's Showcase***, April 2024 and April 2025, Michigan State University.
* Poster presentation: ***Biochemistry and Molecular Biology Scientific Symposium***, May 2024, Michigan State University.
* Oral presentation: ***ACS Spring*** *(COMP Division),* March 2024, New Orleans.
* Oral presentation: ***ACS Spring*** *(BIOT Division),* March 2024, New Orleans.
* Oral presentation: ***Postdoc Symposium****,* Sept 2023, Michigan State University.
* Poster presentation: ***Midwest Undergraduate Computational Chemistry Consortium****,* Aug 2023, Michigan State University.
* Oral presentation: ***MD Simulation: Focus on Methods***, Dec 2022, , Hyderabad, India.
* Oral presentation: ***ACS Fall*** *(COMP Division),* August 2022, Chicago.

* Oral presentation**: *Midwest Protein Folding***, May 2022, University of Notre Dame.
* Oral presentation: ***ACS Spring*** *(COMP Division),* March 2022 (Virtual).
* Oral presentation*: **Molecular Biophysics Supergroup**,* February 2022, Michigan State University.
* Oral presentation: ***Research Scholars Outreach***, January 2020, NCST, Kolkata, India.
* Oral presentation**: *Physical Chemistry Symposium***,** October 2019, IACS, Kolkata, India.

AWARDS & FELLOWSHIPS:

✪ CSIR-UGC National Eligibility Test (NET), all India rank 46 in Chemistry, May 2014: **Entire PhD funding**
✪ Graduate Aptitude Test Engineering (GATE): All India rank 214 in Chemistry, May 2014.
✪ University of Hyderabad M.Sc Entrance Test: All India Rank 5, 2012.
✪ University of Delhi M.Sc Entrance Test: All India Rank 3, 2012.
✪ Recipient of DST-Inspire National Scholarship (2009-2014): **Entire B.Sc and M.Sc tuition funding**
✪ **Submitted an NIH R21 grant proposal as co-investigator (2025).**

VOLUNTARY SERVICES & OUTREACH:

- Member of **American Chemical Society and its COMP division**: Contributed by **presiding** over **oral presentation sessions (2022-2025)**, building a community of postdocs and grad students; member of the **ACS local section**.
- **Reviewer** for *PNAS, Nature Comp. Methods, J Comp. Chem., Royal Soc. Open Sci., LiveComs* etc. scientific journals.
- Member of CMSE Social Events Committee, MSU: **Managing departmental bonding activities and events**.
- Member of MichBio Community: Attending events focused on **biolmedical advances.**
- Member of the Instructor Search Committee, BMB department, MSU.
- Member of team-up postdoc search committee, BMB department, MSU.
- Evaluator of **UURAF, Mid-SURE** etc. multiple conferences in Michigan focused on **outreach activities and promoting undergraduate research,** Michigan State (2022,2023 & 2025)
- Scientific outreach activities in India: Leading collaborations between labs.

REFERENCES:

Dr. Alex Dickson, Professor, email: alexrd@egr.msu.edu
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Specifically for teaching:
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