CURRICULUM VITAE

Bappa Ghosh, Ph.D.

Postdoctoral Researcher,

Department of Biomedical Engineering,

Meta-simulation Non-Equilibrium Processes Group,

University of North Dakota,

USA. ND-58202.

Email: bgchem90@gmail.com bappa.ghosh@und.edu

Phone: (+1)7013147347

Website: https://omegabappa.github.io/

EDUCATION

Aug. 2014–Oct. 2019 Ph.D. in Computational and Theoretical Chemistry,

Department of Chemistry,

Indian Institute of Science Education and Research (IISER) Pune, India.

2011 – 2013 M.Sc. in Chemistry,

Department of Chemistry,

Indian Institute of Technology Kanpur, India.

2008 – 2011 B.Sc. (Hons.) in Chemistry (with distinction),

Department of Chemistry,

Visva-Bharati University, Santiniketan, India.

RESEARCH EXPERIENCES

(Post-Ph.D.)

Sep. 2021 – present Postdoctoral Researcher,

Department of Biomedical Engineering,

University of North Dakota. USA.

Project: Algorithms of estimating entropy production in active matter systems.

Advisor: Prof. Jerome Delhommelle.

Feb. 2020 – Jul. 2021 Postdoctoral Researcher,

School of Chemistry,

IISER Thiruvananthapuram, India-695551.

Project: Investigating the dynamics of organic chromophores in solvents

through atomistic computer simulation.

Advisor: Prof. Mahesh Hariharan.

Oct. 2019 - Feb. 2020 Research Fellow,

Department of Chemistry,

IISER Pune, India-411008.

Project: Effect of solvents on polymer translocation through molecular

dynamics simulation.

Advisor: *Dr. Srabanti Chaudhury*

(Ph.D. work)

Aug. 2014–Oct. 2019 Thesis Title: Some aspects of non-equilibrium polymer translocation dynamics.

Thesis Advisor: Dr. Srabanti Chaudhury

(Pre-Ph.D.)

Jul. 2013 – Jul. 2014 Project Assistant,

Polymers and Advanced Materials Laboratory,

CSIR-National Chemical Laboratory, Pune, Maharashtra, India,

Project: Molecular dynamics study on the growth of carbon dioxide and

methane hydrate from a seed crystal.

Advisor: Dr. Sudip Roy

May 2012 – Jul. 2012 Visiting Summer Project Student,

School of Chemistry,

IISER Thiruvananthapuram, India-695551.

Project: *Molecular modelling of pyrene modified chromophores.*

Advisor: Prof. Mahesh Hariharan

PUBLICATIONS

1. **B. Ghosh**, Ilham Essafri, C. Desgranges, J. Delhommelle, Machine Learning and Active Fluids, (In preparation).

- 2. **B. Ghosh**, Ilham Essafri, C. Desgranges, J. Delhommelle, Designing and Realizing Active Fluids, (In preparation).
- 3. **B. Ghosh**, J. Sarabadani, S. Chaudhury, and T. Ala-Nissila, Pulling a folded polymer through a nanopore, **Journal of Physics: Condensed Matter**, 33, 015101, 2020. [link] [pdf]
- 4. **B. Ghosh**, and S. Chaudhury, Translocation dynamics of an asymmetrically charged polymer through a pore under the influence of different pH conditions, **The Journal of Physical Chemistry B**, 123, 4318-4323, 2019. [link] [pdf]
- 5. P. Nakate, **B. Ghosh**, S. Das, S. Roy, and R. Kumar, Molecular Dynamics Study on Growth of Carbon Dioxide and methane hydrate from a seed crystal, **Chinese Journal of Chemical Engineering**, 27, 2074-2080, 2019. (*invited article*). [link] [pdf]
- 6. **B. Ghosh,** and S. Chaudhury, Influence of the location of attractive polymer—pore interactions on translocation dynamics, **The Journal of Physical Chemistry B**, 122, 360-368, 2018. [link] [pdf]
- 7. J. Sarabadani, **B. Ghosh**, S. Chaudhury, and T. Ala-Nissila, Dynamics of end-pulled polymer translocation through a nanopore, **Europhysics Letters**, 120, 38004, 2017. [link] [pdf]
- 8. **B. Ghosh**, and S. Chaudhury, Fluctuation theorems for total entropy production in generalized Langevin systems, **Physica A: Statistical Mechanics and its Applications**, 466, 133-139, 2017. [link] [pdf]

TEACHING EXPERIENCESS

Teaching Assistant for Chemical Principles I (CHM 101), IISER Pune,

Coordinator: Dr. Arnab Mukherjee,

Teaching Assistant for Statistical Thermodynamics (CHM 422), IISER Pune,

Coordinator: Dr. Srabanti Chaudhury,

Teaching Assistant for Molecular Modelling and Simulation (CHM 436),

IISER Pune, Coordinator: Dr. Arun Venkatnathan,

TALKS/CONFERENCES/WORKSHOPS

Invited Talks

• "Role of Polymer-Pore Interactions in Translocation dynamics" presented in "Soft Matter and Statistical Mechanics 2019", IISER Pune, India.

- "Role of Polymer-Pore Interactions in Translocation dynamics" presented in "Puri Polymer Conference 2018", Puri, India.
- "Influence of the Location of Attractive Polymer-Pore Interactions on Translocation Dynamics" presented in "Chemsymphoria", 2018, IISER Pune, India.

Poster Presentations

- "A comparative study of algorithms to find information entropy in equilibrium and non-equilibrium systems", 2022, APS Physics March Meeting 2022, Chicago, USA.
- "Self-organization in Active Matter: From Living Crystals to Cells and Living Systems", 2021, Annual North Dakota Biomedical Engineering Symposium, University of North Dakota, USA.
- "Polymer Translocation: A few Investigations from Computer Simulations" presented in "Hünfeld 2021: Workshop on Computer Simulation and Theory of Macromolecules", 2021, Max Planck Institute for Biophysical Chemistry, Goettingen, Germany.
- "Pulling a Folded Polymer through a Nanopore" presented in "Frontiers in Ion Channels and Nanopores: Theory, Experiments, and Simulations (FICN2021)", Sapienza University of Rome, Italy.
- "Role of Polymer-Pore Interactions in Translocation dynamics" presented in "Multi-scale Simulation & Mathematical Modelling of Complex Biological Systems 2019", Jawaharlal Nehru University, New Delhi, India.
- "Dynamics of End-pulled polymer Translocation Through a Nanopore" presented in "Society of Polymer Science, India, SPSI-MACRO 2018", IISER Pune, India.
- "Influence of the Location of Attractive Polymer-Pore Interactions on Translocation Dynamics" presented in "Recent Advances in Modeling Rare Events (RARE2017)", Agra, India.
- "End-pulled Polymer Translocation through a Nanopore" presented in "15th Indian Theoretical Chemistry Symposium", 2016, University of Hyderabad, India.
- "Entropy Production Theorems in Systems with Memory" presented in "Physical and Biophysical Chemistry Theory and Experiment", 2015, IIT Bombay, India.

Workshops

- Designed and instructed courses in the "Advanced Molecular Dynamics Simulation: A SAARC Regional Summer School 2021" to train undergraduates, graduate participants through hands-on sessions in Virtual Box, Linux Systems, Grace, gnuplot, scripting, MD in GROMACS.
- Volunteered in the inhouse "Molecular Modeling in Chemistry" workshop on Gaussian, Autodock, MOPAC, molecular modeling, December 2018, IISER Pune, India.

Participations

- "International Conference on Ultrafast Spectroscopy (ICUS2020)", 2020, IISER Thiruvananthapuram, India.
- "14th Indian Theoretical Chemistry Symposium", 2014, CSIR-NCL and IISER Pune, India.

REFERENCES

1. Dr. Srabanti Chaudhury (Thesis Advisor),

Associate Professor,

Department of Chemistry,

Indian Institute of Science Education and

Research Pune, Maharashtra,

India-411008.

E-mail: srabanti@iiserpune.ac.in

Phone: +912025908140

Website: click url

3. **Prof. Jerome Delhommelle**,

Associate Professor,

Department of Biomedical Engineering,

University of North Dakota,

USA, ND-58202

E-mail: jerome.delhommelle@und.edu

Phone: +17017772495 **Website:** *click url*

2. Dr. Arnab Mukherjee,

Associate Professor,

Department of Chemistry,

Indian Institute of Science Education and

Research Pune, Maharashtra,

India-411008.

E-mail: arnab.mukherjee@iiserpune.ac.in

Phone: +912025908051

Website: click url

4. Prof. Mahesh Hariharan,

Professor,

School of Chemistry,

Indian Institute of Science Education and Research Thiruvananthapuram, India-

695551.

E-mail: mahesh@iisertvm.ac.in

Phone: +914712778101

Website: click url