CURRICULUM VITAE

Bappa Ghosh, *Ph.D.*
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RESEARCH INTERESTS

Computational and Theoretical Study of Chemical Systems, Statistical Thermodynamics, Polymer Dynamics, Soft-Condensed Matter, Multiscale-Simulation.

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,
Department of Chemistry,
Visva-Bharati University, Santiniketan, India.

RESEARCH EXPERIENCES

(Post–Ph.D.)

Feb. 2020 – present. **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*

- The solvent effect on polymer translocation was modelled with tuning the intra-chain non-bonded interactions among monomers. The behavior was

studied for a single chain polymer from coarse-grained Langevin dynamics simulation.

(Ph.D. work)

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

Thesis Advisor: *Dr. Srabanti Chaudhury*

Projects:

- **Pore-Driven Polymer translocation**

The influence of polymer-pore interactions on the translocation dynamics using Langevin dynamics simulations was probed. I investigated the effect of the strength and location of the polymer-pore interaction using nanopores that are partially charged either at the entry or the exit or on both sides of the pore. The simulation results were rationalized by a qualitative analysis of the free energy landscape for polymer translocation.

In another work, the translocation of a polymer with oppositely charged segments at both ends was looked into in the presence of a pH gradient using Langevin dynamics simulations. My simulation results captured many features observed in experiments. The results were also explained qualitatively by calculating the free-energy change of the polymer chain during the translocation process.

- **End-pulled Translocation**

I studied the translocation dynamics of a polymer chain forced through a nanopore by an external force on its head monomer on the *trans* side. The simulation results indicated to include friction arising from the *trans* side sub chain to generalize the iso-flux tension propagation (IFTP) theory.

In another work, I looked into the translocation dynamics of a folded linear polymer which is pulled through a nanopore by an external force. My molecular dynamics simulation (MD) helped to extensively bench-mark the theory. Using the assumption of equal monomer flux of both branches by MD simulations, the analytical equations of motion for both branches were derived. The translocation dynamics was characterized in detail from the average waiting time and its scaling form.

- **Entropy Production Calculation**

I calculated the total entropy production of a colloidal particle embedded in a non-Markovian heat bath driven by a time-dependent force in a harmonic potential. The dynamics of the system was modelled by the generalized Langevin equation with coloured noise. The distribution function of entropy production was calculated which showed the detailed fluctuation theorem contains a renormalized temperature term in a non-Markovian thermal bath.

(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*

- The spontaneous growth of CO_2 and CH_4 clathrate hydrate growth were studied from a seed hydrate crystal. Order parameter of water and clathrate states were calculated to monitor the growth of the crystal phase through all-atomistic molecular dynamics simulation.

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*

- The pyrene modified G-quadruplex was studied through atomistic molecular dynamics simulation to find out the dynamical properties of chromophore tag in solvents.

PUBLICATIONS

1. **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]

2. **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]

3. 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]

4. **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]

5. 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]

6. **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

2015 (Fall) **Teaching Assistant** for Chemical Principles I (CHM 101), IISER Pune,
Coordinator: Dr. Arnab Mukherjee,

2016 (Spring) **Teaching Assistant** for Statistical Thermodynamics (CHM 422), IISER Pune,
Coordinator: Dr. Srabanti Chaudhury,

2016 (Fall) **Teaching Assistant** for Molecular Modelling and Simulation (CHM 436), IISER Pune, Coordinator: Dr. Arun Venkatnathan,

AWARDS/FELLOWSHIPS/ACHIEVEMENTS

- Qualified in all India Graduate Aptitude Test Engineering (GATE 2013).
- Selected for Merit-cum-Means Scholarship at IIT Kanpur during M.Sc.
- Qualified in the all India Joint Admission Test for M.Sc. (IIT-JAM 2011).
- Selected for National Merit Scholarship for 41th rank in West Bengal (India) State Board.

CONFERENCES

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

- "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

- 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.

SKILLS

- Performing molecular dynamic simulations (all-atomistic and coarse-grained) and analyzing data, free energy calculations, Langevin dynamics.
- Computational software: GROMACS, LAMMPS, VMD, xmgrace, molden,
- Programming Languages: FORTRAN77, C, Python, HTML, CSS, JavaScript and Bash scripting.
- Application software: Inkscape, Blender, Gimp, MS-Office, Latex.

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
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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
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3. **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
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4. **Prof. Tapio Ala-Nissilä,**
   Professor,
   Department of Applied Physics,
   Aalto University,
   Finland.
   E-mail: tapio.ala-nissila@aalto.fi
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