

## CURRICULUM VITAE

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### **Bappa Ghosh, *Ph.D.***

Postdoctoral Researcher,  
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### 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. Ilham Essafri, **B. Ghosh**, 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 EXPERIENCES

2015 (Fall)	<b>Teaching Assistant</b> for Chemical Principles I (CHM 101), IISER Pune, Coordinator: Dr. Arnab Mukherjee,
2016 (Spring)	<b>Teaching Assistant</b> for Statistical Thermodynamics (CHM 422), IISER Pune, Coordinator: Dr. Srabanti Chaudhury,
2016 (Fall)	<b>Teaching Assistant</b> 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.  
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2. **Dr. Arnab Mukherjee**,  
Associate Professor,  
Department of Chemistry,  
Indian Institute of Science Education and  
Research Pune, Maharashtra,  
India-411008.  
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3. **Prof. Jerome Delhommelle**,  
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4. **Prof. Mahesh Hariharan**,  
Professor,  
School of Chemistry,  
Indian Institute of Science Education and  
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