

Samyabrata Chatterjee (CV)

CONTACT INFORMATION

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Google Scholar: <https://shorturl.at/fSEGT>

EDUCATION

PhD Candidate in Chemical Engineering, Sep 2020 - Dec 2025

- Dissertation Topic: “ Design of high energy density supercapacitors using molecular dynamics simulations ”
- Advisor: Dr. Monojit Chakraborty
GPA: 8.80/10

M.Tech Candidate in Chemical Engineering, Aug 2018 - July 2020

- Dissertation Topic: “A Molecular Dynamics Simulations Study of Polyelectrolyte Adsorption on Charged Surfaces”
- Advisor: Dr. Mithun Radhakrishna
GPA: 7.67/10

B.Tech Heritage Institute of Technology, Kolkata, India Aug 2013 - July 2017

- Dissertation Topic: “Treatment of simulated wastewater using Sono-Fenton process”
- Advisor: Abhyuday Mallick
GPA: 8.66/10

Higher Secondary Examination, Ramakrishna Mission Vidyalaya , Aug 2013
Narendrapur, Kolkata, India
Percentage: 84.40

Secondary Examination, Ramakrishna Mission Vidyalaya , July 2011
Narendrapur, Kolkata, India
Percentage: 89.37

RESEARCH INTERESTS

Computational Chemistry, AI/ML based force field design for Molecular Dynamics simulations, Molecular Dynamics Simulations, Surface-particle interactions, Supercapacitors, Statistical Mechanics, Polymer Physics, Microfluidics, Water droplet dynamics, Advanced Oxidation Processes for Water Treatment

RESEARCH SKILLS

- Molecular Dynamics Simulation packages like using LAMMPS and NAMD
- Softwares like VMD, Packmol, Avogadro
- Experienced in using High Performance Computing clusters
- Knowledge in programming languages like C++, Python for performing Data Analysis

WORK EXPERIENCE

- Mercor (August 2025 - November 2025)
 - (1) Chemistry labelling expert
 - (2) Chemistry audit expert
- Prime Minister Research Fellow at Indian Institute of Technology, Kharagpur (September 2020 - current)
 - (1) Molecular Dynamics study regarding water droplet interaction of crystal surfaces
 - (2) Molecular Dynamics study regarding patterned polyelectrolyte as supercapacitor electrolytes
 - (3) Multiscale investigation study of liquid imbibition on an electrodeposited rough surface

(4) Molecular Perspectives on the Multilayered polyelectrolyte-based electrodes performance in supercapacitors

- Masters of Technology at Indian Institute of Technology, Gandhinagar (September 2020 - current)
 - (1) Molecular Dynamics study regarding polyelectrolyte adsorption on charged surface
- Summer training at ITC limited Paper Boards Specialty paper division on “Overview of WTP and ETP” (June, 2016 – July, 2016)
 - (1) Studied about the various layouts of a water treatment plant and an effluent treatment plant
 - (2) Hands-on experience of various methods of effluent treatment
- Summer Training at Kolkata Municipal Corporation on “Kolkata Water Supply Transmission and Distribution” (June, 2015 – July, 2015)
 - (1) Surveyed about the water supply and distribution in the city of Kolkata
 - (2) Learnt about the water treatment procedures followed by the corporation (monitoring BOD, COD, bacteria removal technologies)

PUBLICATIONS

- Chatterjee, S., Singh, A., Chakraborty, M. (2023). Molecular Insights into the Effect of Crystal Planes on Droplet Wetting. *Langmuir*, 39(13), 4789-4798.
- Chatterjee, S., Paras, Hu, H., Chakraborty, M. (2023). A Review of Nano and Microscale Heat Transfer: An Experimental and Molecular Dynamics Perspective. *Processes*, 11(9), 2769.
- Chatterjee, S., Ganesh, P. S., Chakraborty, M. (2024). Molecular insight into sequence-defined polyelectrolytes for energy storage devices. *Electrochimica Acta*, 491, 144306.
- Panda, I., Chatterjee, S., Chakraborty, M., DasGupta, S. (2024). Multiscale Investigation of Liquid Imbibition on an Electrodeposited Rough Surface. *Langmuir*, 40(49), 25849-25861.

CONFERENCE PRESENTATION

- International Conferences on Super-capacitors Energy Storage and Applications (ICSEA-2019) Centre for Materials for Electronics Technology (C-MET)
- Complex Fluids Symposium 2022 (CompFlu - 2022)

AWARD

- Prime Minister's Research Fellow (2021-present)