

Abhishek Kumar Gupta, Ph.D.

MB-203, Department of Chemical Engineering
IIT Kharagpur
Kharagpur-721302, West Bengal, India

Email: akg@che.iitkgp.ac.in
Contact No: +91-3222214586

Education

- **Ph.D. - Chemical Engineering** July 2013-March 2019
Indian Institute of Technology (IIT) Madras, Chennai, India
Advisor: Prof. Upendra Natarajan

- **Masters in Engineering (ME) - Chemical Engineering** June 2013
Jadavpur University, Kolkata, India
Advisor: Prof. Rajat Chakraborty
Aggregate CGPA: 8.22/10

- **B.Tech - Chemical Engineering** June 2011
SASTRA University, Thanjavur, India
Faculty Advisor: Prof. Ponnusami V
Aggregate CGPA: 9.01/10

Research Interests

- Molecular dynamics Simulations
- Molecular Simulations
- Stimuli-responsive polymers
- Novel smart polymeric materials
- Self-assembly of block copolymers

Experience

1. **Guest Faculty, National Institute of Technology Arunachal Pradesh, Yupia, State: Arunachal Pradesh, India** (Jan 7th, 2019 – Feb 19, 2019) – Courses Taken: Mechanical Unit Operations, Process Equipment Design-II, Numerical Methods Laboratory
2. **Assistant Professor, Pandit Deendayal Energy University (Formerly Pandit Deendayal Petroleum University), Gandhinagar, State: Gujarat, India** (March, 2019 – November, 2023) – Theory Courses: Mechanical Unit Operations, Heat Transfer, Polymer Science and Technology, Material Modeling and Simulation Techniques (M.Tech.). Lab courses: Mechanical Operations Lab, Heat Transfer Lab; Environmental Engineering Lab.
3. **Assistant Professor, Department of Chemical Engineering, IIT Kharagpur, WB, India** (November 2023 – To Date)

Publications

1. Rajat Chakraborty, **Abhishek Kumar Gupta**, R. Chowdhury. Conversion of slaughterhouse and poultry farm animal fats and wastes to biodiesel: Parametric sensitivity and fuel quality assessment. *Renewable and Sustainable Energy Reviews*. **2014**, 29, 120-134.
2. **Abhishek Kumar Gupta**, U. Natarajan. Tacticity effect on conformational structure and hydration of poly(methacrylic acid) in aqueous solution. *Molecular Simulation*. **2016**, 42(9), 725-736.
3. **Abhishek Kumar Gupta**, U. Natarajan. Anionic polyelectrolyte poly (acrylic acid)(PAA) chain shrinkage in water–ethanol solution in presence of Li⁺ and Cs⁺ metal ions studied by molecular dynamics simulations. *Molecular Simulation*. **2017**, 43(8), 625-637.
4. **Abhishek Kumar Gupta**, U. Natarajan. Structure and dynamics of *atactic* Na⁺-poly(acrylic acid) PAA polyelectrolyte in aqueous solution in dilute, semi-dilute and concentrated regimes. *Molecular Simulation*. 2019, 45(11), 876-895.
5. Yogendra Kumar, **Abhishek Kumar Gupta**, U. Natarajan. Conformational studies of stereoregularisomers of poly(acrylic acid) in dilute aqueous solutions using molecular dynamics simulation study. *Molecular Simulation*. 2020, 46(18), 1483-1499.
6. **Abhishek Kumar Gupta**, Combined Salt Concentration and Degree-of-Ionization Effect on the Structure of Poly(methacrylic acid) in Aqueous Solutions as Revealed by Molecular Dynamics Simulations, *Industrial & Engineering Chemistry Research* **2021**, 60, 13, 4806–4819.
7. **Abhishek Kumar Gupta**, Siddhant Gohil, Insights into Structural difference between Sodium-Polyacrylate PAA and Sodium-Polymethacrylate PMA in salt solutions, *Journal of Materials Science* **2022**, 57, 10569–10584.
8. **Abhishek Kumar Gupta**, Sr²⁺ and Ba²⁺ salts induced conformational structure of sodium polyacrylate PAA investigated by molecular dynamics simulations. *Computational Materials Science* **2022**, 211, 111541
9. **Abhishek Kumar Gupta**, Salt Ions Induced Transport Properties Of Poly(Methacrylic Acid) PMA In Aqueous Solutions Studied By Molecular Dynamics Simulations. *Materials Today: Proceedings* **2021**, 44, 2380-2385.
10. **Abhishek Kumar Gupta**, Molecular dynamics simulations studies of transport properties of sodium-(polymethacrylate)(Na⁺-PMA) in aqueous solutions–Effect of salt concentration. *Materials Today: Proceedings* **2021**, 43, 3085-3090.

Book Chapters

1. **Abhishek Kumar Gupta**. Modeling and molecular simulation methods for CO₂ capture. In Emerging Carbon Capture Technologies 2022 Jan 1 (pp. 347-369). Elsevier.
2. Jagadeeshwar Kodavaty, Suresh Kumar Yatirajula, **Abhishek Kumar Gupta**, and Rejeswara Reddy Erva. Characteristics of Hydrogels. Hydrogels Fundamentals to Advance Energy Applications, CRC Press. pp: 83-102.

Sponsored Projects

1. **Project Title:** Amphiphilic Thermoresponsive Block-copolymer Hydrogels and their Interactions with Carboxymethyl Cellulose for Efficient Ocular Drug Delivery Applications. Funding Agency: **SERB**; Role: PI; Sanctioned amount: 18.30 lakhs.

Ph.D. Thesis Supervision

Sr. No.	Name of the Research Scholar	Ongoing/Completed	Area of research
1	Parag Choudhury	Ongoing	Block-copolymer self-assembly

M.Tech/ Master's Thesis Supervision

Sr. No.	Name of Student	Ongoing/Completed	Ongoing/year of completion
1	Saleh Hussein	Completed	2023
2	Abdulkarem Alqardai	Completed	2023
3	Kishan Agarwal	Completed	2022
3	Siddhant Gohil	Completed	2021
4	Meet Vaidya	Completed	2020

International Conference Presentations

1. **Abhishek Kumar Gupta**, U. Natarajan “Effect of tacticity and degree of neutralization on chain dimension of Poly-(methacrylic acid) in dilute aqueous solution” Third International Conference on Polymer Processing and Characterization ICPPC-2014, Mahatma Gandhi University, Kottayam, India. 11-13 Oct (2014).
2. **Abhishek Kumar Gupta**, U. Natarajan “Effect of tacticity on chain dimension of Poly-(methacrylic acid) in dilute aqueous solution” Macro-2015 International Symposium on Polymer Science and Technology, Indian Association for Cultivation of Science, Kolkata, India. 23-26 Jan (2015).
3. **Abhishek Kumar Gupta**, U. Natarajan “Counterion specific collapse of fully ionized PAA in water- ethanol mixture in presence of Li⁺ and Cs⁺ alkali metal cations-A molecular

dynamics simulation study ” International Conference on Nanostructured Polymeric Materials and Polymer Nanocomposites (ICNPM-2015), Mahatma Gandhi University, Kottayam, India. 13-15 Nov (2015).

4. **Abhishek Kumar Gupta**, U. Natarajan “Collapse of PAA in water-ethanol mixture in presence of Li^+ and Cs^+ alkali metal cations-A molecular dynamics simulation study ” International Conference on Frontiers at the Chemistry – Allied Sciences Interface (FCASI-2016), 25-26 April (2016) Jaipur, India.
5. **Abhishek Kumar Gupta**, U. Natarajan “Counterion specific collapse of fully ionized PAA in water- ethanol mixture in presence of Li^+ and Cs^+ alkali metal cations-A molecular dynamics simulation study ” 6th International Conference on Functional Electroceramics and Polymers (ICEP-2017), Feb. 20-22 (2017) IIT Kharagpur, India.
6. **Abhishek Kumar Gupta**, U. Natarajan. “Molecular dynamics simulation studies of structure and dynamics of Poly(acrylic) acid In semi-dilute concentration regime” 9th Conference of Asian Consortium of Computational Materials Science (ACCMS-9) Meeting, Aug. 8- 11 (2017), Kuala Lumpur, Malaysia.
7. **Abhishek Kumar Gupta**, U. Natarajan. “Conformation structure, dynamics and thermodynamics of Poly(acrylic) acid In semi-dilute concentration regime as investigated by molecular dynamics simulations study” at Asia-Pacific Conference of Theoretical and Computational Chemistry (APCTCC 8) Meeting, Dec. 15-17 (2017), IIT Bombay, Mumbai. India.
8. **Abhishek Kumar Gupta**, U. Natarajan. “Effect of Co-solvent (Ethanol) and PAA concentration on the structure and dynamics of sodium-polyacrylate (Na^+ -PAA) in solutions investigated by MD Simulations” at Physical Aspects of Polymer Science 2019, Sep. 11-13 (2019), IOP Polymer Physics Group, UK.
9. **Abhishek Kumar Gupta**, Molecular Dynamics Simulations Studies of Structure and Dynamics of Polyelectrolytes in Solutions, International Conference on Macromolecules-2020, Kottayam, Kerala, India.
10. **Abhishek Kumar Gupta**, Salt Ions Induced Transport Properties Of Poly(Methacrylic Acid) PMA In Aqueous Solutions Studied By Molecular Dynamics Simulations, ICMPC-2020, IIT Indore, M.P., India.
11. **Abhishek Kumar Gupta**, Molecular dynamics simulations studies of transport properties of sodium-(polymethacrylate) (Na^+ -PMA) in aqueous solutions–Effect of salt concentration, CRMSC 2021, Manipal University Jaipur, Jan 11-12, 2021, India.
12. **Abhishek Kumar Gupta**, Hydrogen bond dynamics of polymethacrylic acid and sodium polymethacrylate in aqueous salt solutions investigated by molecular simulations, MMETFP 2021, PDEU Gandhinagar, Nov 19-21, 2021, India.
13. **Abhishek Kumar Gupta**, Structural aspects of charged polyelectrolytes in salt solutions – An atomistic simulation study, ICTSGS 2021, Yamagata University Japan, Nov 29-30, 2021, India.
14. **Abhishek Kumar Gupta**, Hydrogen bond dynamics of polymethacrylic acid and sodium polymethacrylate in aqueous salt solutions investigated by molecular simulations, MMETFP 2021, PDEU Gandhinagar, Nov 19-21, 2021, India.

15. **Abhishek Kumar Gupta**, Structure and Dynamics of anionic polyelectrolytes in salt solutions - An atomistic simulation study, Chemsart 2022, NIT Rourkela, December 16-18, 2022.
16. **Abhishek Kumar Gupta**, Structure and Dynamics of anionic polyelectrolytes in salt solutions - An atomistic simulation study, RAMCC 2023, Dibrugarh University, March 1-3, 2023.

Awards and Accolades

- **Best Oral Presentation Award**, International Conference on Frontiers at the Chemistry – Allied Sciences Interface (FCASI-2016), 25-26 April (2016) at University of Rajasthan in Department of Chemistry, Jaipur, India, “Conformational structure of PAA in water-ethanol mixture in presence of Li^+ and Cs^+ alkali metal cations-A molecular dynamics simulation study”.
- **Young Scientist Award for the Best Poster**, 6th International Conference on Functional Electroceramics and Polymers (ICEP-2017), Feb. 20-22 (2017) IIT Kharagpur, India, “Counterion specific collapse of fully ionized PAA in water-ethanol mixture in presence of Li^+ and Cs^+ alkali metal cations-A molecular dynamics simulation study”.
- **Best Oral Presentation Award at CRMSC-2021** organized by Department of Chemistry and Biosciences, School of basic Sciences, Manipal University Jaipur, Jan-11-12, 2021
- **Dean’s list Award** for being in top 2% of the UG Batch in terms of academic performance during the II year (2008-2009) of the four year B.Tech. Degree Programme (SASTRA University).

Membership of Professional Bodies

- Member-American Chemical Society (ACS)